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## Benzyl anion abstraction from a (beta-diiminato)Fe(II) benzyl complex

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### # 3. TITLE AND AUTHOR LIST

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Benzyl anion abstraction from a (\B-diiminato)Fe(II) benzyl complex  
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\_publ\_section\_references  
;

Beurskens, P.T., Beurskens, G., Gelder, R. de    Garcia-Granda, S.  
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;

\_publ\_section\_figure\_captions

;

Fig. 1. Chemical structural diagram (scheme 1) of the title compound

Fig. 2. Perspective PLUTO drawing of the molecule illustrating the  
configuration and the adopted numbering scheme.

Fig. 3. Molecular packing viewed down unit cell axes.

Fig. 4. Perspective ORTEP drawing of the title compound.  
Displacement ellipsoids for non-H are represented at the 50%  
probability level.

The H-atoms have been omitted to improve clarity.

;

#=====

data\_c77h108f

\_database\_code\_CSD            185602

\_audit\_creation\_date            '2001-08-27 14:56:42'  
\_audit\_creation\_method        'PLATON <TABLE ACC> option'  
\_audit\_update\_record

;

?

;

#=====

# 5. CHEMICAL DATA

\_chemical\_name\_systematic

;

?

;

\_chemical\_name\_common            ?  
\_chemical\_melting\_point           ?  
\_chemical\_formula\_moiety  
'2(C36 H48 Fe N2), C5 H12'  
\_chemical\_formula\_structural       ?  
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)<sub>3</sub>, (C6 N6 Cr 3-)<sub>2</sub>, 2(H2 O)'  
\_chemical\_formula\_sum  
'C77 H108 Fe2 N4'  
\_chemical\_formula\_weight           1201.37  
\_chemical\_compound\_source        'see text'

loop\_

\_atom\_type\_symbol

\_atom\_type\_description

\_atom\_type\_scatter\_dispersion\_real

```

_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
N   N   0.0061   0.0033
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Fe Fe   0.3463   0.8444
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H   H   0.0000   0.0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C   C   0.0033   0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

```

#=====

## # 6. CRYSTAL DATA

```

_symmetry_cell_setting      Monoclinic
_symmetry_space_group_name_Hall '-P 2ybc'
_symmetry_space_group_name_H-M 'P 21/c'

```

```

loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x,1/2+y,1/2-z
-x,-y,-z
x,1/2-y,1/2+z

```

```

_cell_length_a      15.3319(9)
_cell_length_b      20.652(1)
_cell_length_c      22.408(1)
_cell_angle_alpha    90
_cell_angle_beta     90.781(1)
_cell_angle_gamma    90
_cell_volume         7094.5(6)
_cell_formula_units_Z 4

```

```

_cell_measurement_temperature 125(1)
_cell_measurement_reflns_used 7023
_cell_measurement_theta_min 2.44
_cell_measurement_theta_max 28.98
_cell_special_details
;

```

The final unit cell was obtained from the xyz centroids of 7023 reflections after integration using the SAINT software package (Bruker, 2000).

```

_exptl_crystal_description 'platelet'
_exptl_crystal_colour      'red'
_exptl_crystal_size_max    0.45
_exptl_crystal_size_mid    0.40
_exptl_crystal_size_min    0.12
_exptl_crystal_size_rad    ?
_exptl_crystal_density_meas ?
_exptl_crystal_density_diffn 1.125
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000       2600
_exptl_absorpt_coefficient_mu 0.452
_exptl_absorpt_correction_type 'Multi-Scan'
_exptl_absorpt_process_details '(SADABS, Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min 0.8226
_exptl_absorpt_correction_T_max 0.9478

```

#=====

## # 7. EXPERIMENTAL DATA

```
_exptl_special_details
;
?
;

_diffrn_ambient_temperature      125(1)
_diffrn_radiation_wavelength     0.71073
_diffrn_radiation_type           MoK\alpha
_diffrn_radiation_source         'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator   'parallel mounted graphite'
_diffrn_radiation_detector
;
CCD area-detector
;
_diffrn_measurement_device_type
;
Bruker Smart Apex
;
_diffrn_measurement_method       'phi and omega scans'
_diffrn_special_details
;
Crystal into the cold nitrogen stream of the low-temperature
unit (KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean  '4096x4096 / 62x62 (binned 512)'

_diffrn_standards_number         ?
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time  ?

loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number            44924
_diffrn_reflns_av_R_equivalents  0.0276
_diffrn_reflns_av_sigmaI/netI    0.0398
_diffrn_reflns_limit_h_min       -21
_diffrn_reflns_limit_h_max       16
_diffrn_reflns_limit_k_min       -28
_diffrn_reflns_limit_k_max       28
_diffrn_reflns_limit_l_min       -27
_diffrn_reflns_limit_l_max       30
_diffrn_reflns_theta_min         2.38
_diffrn_reflns_theta_max         29.75
_diffrn_measured_fraction_theta_max 0.897
_diffrn_reflns_theta_full        29.75
_diffrn_measured_fraction_theta_full 0.897

_diffrn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o \sim ^2$ 
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
_reflns_number_total            18149
_reflns_number_gt               13810
```

```

_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'SMART, Bruker Version 5.168, 2000'
_computing_cell_refinement        'SAINT, Bruker Version 6.02A, 2000'
_computing_data_reduction        'XPREP, Bruker Version 5.1/NT, 2000'
_computing_structure_solution
;
DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2001)
PLATON (Spek, 1994)
;
_computing_publication_material
;
PLATON (Spek, 1990)
SHELXL (Sheldrick, 1997)
;

#=====

# 8. REFINEMENT DATA

_refine_special_details
;
Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type           full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
'calc w=1/[s2(Fo2)+(0.0612P)2+0.8899P] where P=(Fo2+2Fc2)/3'
_refine_ls_solution_primary      direct
_refine_ls_solution_secondary    difmap
_refine_ls_solution_hydrogens    geom
_refine_ls_hydrogen_treatment    mixed
_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
_refine_ls_abs_structure_details ?
_refine_ls_abs_structure_Flack   ?
_refine_ls_number_reflns        18149
_refine_ls_number_parameters     1181
_refine_ls_number_restraints     0
_refine_ls_number_constraints    ?
_refine_ls_R_factor_all          0.0623
_refine_ls_R_factor_gt           0.0430
_refine_ls_wR_factor_ref         0.1134
_refine_ls_wR_factor_gt          0.1044
_refine_ls_goodness_of_fit_ref   1.022
_refine_ls_restrained_S_all      1.022
_refine_ls_shift/su_max          0.002
_refine_ls_shift/su_mean         0.000

_refine_diff_density_max         0.525

```

```
_refine_diff_density_min      -0.239
_refine_diff_density_rms      0.056
_vrn_publ_code_void_volume    0.000
_vrn_publ_code_meas_time      7.95
```

#####

# # 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
Fe11 Fe Uani 0.14330(1) 0.22131(1) 0.18920(1) 1.000 0.0218(1) . .
N11 N Uani 0.23555(7) 0.16055(5) 0.16336(5) 1.000 0.0196(3) . .
N12 N Uani 0.19949(7) 0.23957(6) 0.26752(5) 1.000 0.0205(3) . .
C11 C Uani 0.16232(10) 0.06468(7) 0.12312(7) 1.000 0.0269(5) . .
C12 C Uani 0.13671(11) 0.02771(8) 0.07379(9) 1.000 0.0360(5) . .
C13 C Uani 0.15822(12) 0.04613(9) 0.01654(9) 1.000 0.0415(6) . .
C14 C Uani 0.20704(12) 0.10119(9) 0.00711(8) 1.000 0.0377(6) . .
C15 C Uani 0.23603(10) 0.13947(7) 0.05490(7) 1.000 0.0273(5) . .
C16 C Uani 0.21330(9) 0.12046(7) 0.11268(7) 1.000 0.0222(4) . .
C17 C Uani 0.13647(12) 0.04582(8) 0.18572(8) 1.000 0.0356(5) . .
C18 C Uani 0.20557(17) 0.00482(17) 0.21641(15) 1.000 0.0734(11) . .
C19 C Uani 0.04829(14) 0.01232(13) 0.18890(12) 1.000 0.0517(8) . .
C110 C Uani 0.28743(11) 0.20086(8) 0.04259(8) 1.000 0.0309(5) . .
C111 C Uani 0.22794(15) 0.25221(10) 0.01405(10) 1.000 0.0459(7) . .
C112 C Uani 0.36667(14) 0.18819(11) 0.00304(10) 1.000 0.0439(7) . .
C113 C Uani 0.31267(9) 0.15372(6) 0.19074(6) 1.000 0.0207(4) . .
C114 C Uani 0.38180(11) 0.11102(8) 0.16365(8) 1.000 0.0284(5) . .
C115 C Uani 0.33433(9) 0.18472(7) 0.24473(7) 1.000 0.0212(4) . .
C116 C Uani 0.28122(9) 0.22184(7) 0.28189(7) 1.000 0.0213(4) . .
C117 C Uani 0.31907(12) 0.24099(10) 0.34160(8) 1.000 0.0317(5) . .
C118 C Uani 0.14870(9) 0.27243(7) 0.31197(7) 1.000 0.0230(4) . .
C119 C Uani 0.14852(10) 0.34045(7) 0.31438(7) 1.000 0.0266(4) . .
C120 C Uani 0.09698(11) 0.37085(9) 0.35697(8) 1.000 0.0334(5) . .
C121 C Uani 0.04713(11) 0.33496(10) 0.39611(8) 1.000 0.0374(6) . .
C122 C Uani 0.04736(11) 0.26859(10) 0.39303(8) 1.000 0.0350(5) . .
C123 C Uani 0.09765(10) 0.23554(8) 0.35117(7) 1.000 0.0277(5) . .
C124 C Uani 0.20128(11) 0.38125(8) 0.27166(8) 1.000 0.0334(5) . .
C125 C Uani 0.14180(16) 0.41505(12) 0.22648(11) 1.000 0.0507(8) . .
C126 C Uani 0.26009(19) 0.43015(13) 0.30458(14) 1.000 0.0628(10) . .
C127 C Uani 0.09514(12) 0.16200(9) 0.34823(8) 1.000 0.0356(5) . .
C128 C Uani 0.1103(2) 0.13070(12) 0.40909(11) 1.000 0.0570(9) . .
C129 C Uani 0.00957(18) 0.13855(14) 0.32077(15) 1.000 0.0641(10) . .
C130 C Uani 0.03108(11) 0.25222(8) 0.14824(9) 1.000 0.0327(5) . .
C131 C Uani -0.02700(10) 0.19824(8) 0.12902(8) 1.000 0.0304(5) . .
C132 C Uani -0.09998(11) 0.18042(9) 0.16208(8) 1.000 0.0372(6) . .
C133 C Uani -0.15343(12) 0.12970(10) 0.14458(10) 1.000 0.0441(7) . .
C134 C Uani -0.13655(12) 0.09491(10) 0.09338(9) 1.000 0.0429(6) . .
C135 C Uani -0.06439(11) 0.11144(9) 0.06005(8) 1.000 0.0377(6) . .
C136 C Uani -0.01050(11) 0.16197(9) 0.07746(8) 1.000 0.0327(5) . .
Fe21 Fe Uani 0.64257(1) 0.29646(1) 0.18208(1) 1.000 0.0220(1) . .
N21 N Uani 0.73430(8) 0.35271(6) 0.14853(5) 1.000 0.0212(3) . .
N22 N Uani 0.70238(8) 0.28683(6) 0.26031(5) 1.000 0.0216(3) . .
C21 C Uani 0.66531(10) 0.43976(7) 0.08984(7) 1.000 0.0251(4) . .
C22 C Uani 0.63682(11) 0.46300(8) 0.03475(8) 1.000 0.0314(5) . .
```



C23 C Uani 0.65414(12) 0.43003(8) -0.01735(8) 1.000 0.0328(5) . .  
 C24 C Uani 0.70199(11) 0.37317(8) -0.01520(7) 1.000 0.0296(5) . .  
 C25 C Uani 0.73222(9) 0.34767(7) 0.03859(7) 1.000 0.0237(4) . .  
 C26 C Uani 0.71255(9) 0.38118(7) 0.09142(6) 1.000 0.0213(4) . .  
 C27 C Uani 0.64420(12) 0.47774(8) 0.14605(8) 1.000 0.0326(5) . .  
 C28 C Uani 0.54748(16) 0.47719(15) 0.15852(13) 1.000 0.0608(9) . .  
 C29 C Uani 0.6761(3) 0.54779(12) 0.14142(14) 1.000 0.0732(12) . .  
 C210 C Uani 0.78321(11) 0.28437(8) 0.03876(7) 1.000 0.0282(5) . .  
 C211 C Uani 0.72358(15) 0.22794(9) 0.02000(12) 1.000 0.0458(7) . .  
 C212 C Uani 0.86291(13) 0.28795(11) -0.00177(9) 1.000 0.0415(6) . .  
 C213 C Uani 0.81173(9) 0.36372(7) 0.17446(7) 1.000 0.0226(4) . .  
 C214 C Uani 0.87821(11) 0.40425(9) 0.14236(8) 1.000 0.0302(5) . .  
 C215 C Uani 0.83542(9) 0.33956(7) 0.23094(7) 1.000 0.0240(4) . .  
 C216 C Uani 0.78405(9) 0.30579(7) 0.27193(7) 1.000 0.0236(4) . .  
 C217 C Uani 0.82550(12) 0.29105(10) 0.33197(8) 1.000 0.0348(6) . .  
 C218 C Uani 0.64991(9) 0.26040(7) 0.30732(6) 1.000 0.0229(4) . .  
 C219 C Uani 0.63934(9) 0.19306(8) 0.31229(7) 1.000 0.0254(4) . .  
 C220 C Uani 0.58296(10) 0.16963(9) 0.35570(7) 1.000 0.0313(5) . .  
 C221 C Uani 0.54017(11) 0.21108(9) 0.39399(8) 1.000 0.0350(5) . .  
 C222 C Uani 0.55100(11) 0.27698(9) 0.38846(8) 1.000 0.0333(5) . .  
 C223 C Uani 0.60508(10) 0.30332(8) 0.34501(7) 1.000 0.0284(5) . .  
 C224 C Uani 0.68765(11) 0.14586(8) 0.27263(7) 1.000 0.0283(5) . .  
 C225 C Uani 0.74828(15) 0.10130(12) 0.30911(10) 1.000 0.0470(7) . .  
 C226 C Uani 0.62495(14) 0.10545(10) 0.23437(10) 1.000 0.0428(6) . .  
 C227 C Uani 0.61223(12) 0.37647(9) 0.33897(8) 1.000 0.0379(6) . .  
 C228 C Uani 0.64744(19) 0.40796(12) 0.39607(11) 1.000 0.0549(8) . .  
 C229 C Uani 0.5249(2) 0.40616(14) 0.32104(15) 1.000 0.0652(10) . .  
 C230 C Uani 0.52917(11) 0.25646(8) 0.15081(8) 1.000 0.0295(5) . .  
 C231 C Uani 0.46934(10) 0.30432(7) 0.12190(7) 1.000 0.0268(5) . .  
 C232 C Uani 0.39492(11) 0.32747(9) 0.15076(8) 1.000 0.0352(5) . .  
 C233 C Uani 0.34033(13) 0.37260(9) 0.12397(10) 1.000 0.0428(6) . .  
 C234 C Uani 0.35764(12) 0.39634(9) 0.06751(9) 1.000 0.0393(6) . .  
 C235 C Uani 0.43116(11) 0.37441(8) 0.03842(8) 1.000 0.0335(5) . .  
 C236 C Uani 0.48592(10) 0.32928(8) 0.06503(7) 1.000 0.0280(5) . .  
 C31 C Uani 0.1291(5) 0.4819(4) 0.0776(3) 0.500 0.068(3) . .  
 C32 C Uani 0.0884(3) 0.5140(2) 0.02198(19) 0.500 0.0456(12) . .  
 C33 C Uani -0.0023(5) 0.4893(3) 0.0078(3) 0.500 0.037(2) . .  
 C34 C Uani -0.0465(3) 0.5212(2) -0.04547(19) 0.500 0.0482(14) . .  
 C35 C Uani -0.1368(4) 0.4959(4) -0.0563(3) 0.500 0.068(3) . .  
 C41 C Uani 0.6194(11) 0.0424(5) 0.0741(7) 0.500 0.093(5) . .  
 C42 C Uani 0.5767(3) -0.0038(2) 0.03031(18) 0.500 0.0463(14) . .  
 C43 C Uani 0.4877(5) 0.0088(4) 0.0011(4) 0.500 0.036(2) . .  
 C44 C Uani 0.4591(3) -0.0439(2) -0.04256(18) 0.500 0.0479(14) . .  
 C45 C Uani 0.3811(10) -0.0377(8) -0.0663(7) 0.500 0.126(6) . .  
 H111' H Uiso 0.2603(13) 0.2894(10) 0.0046(9) 1.000 0.047(6) . .  
 H111" H Uiso 0.1767(13) 0.2641(9) 0.0412(9) 1.000 0.043(5) . .  
 H112' H Uiso 0.4004(13) 0.2281(10) -0.0007(9) 1.000 0.044(6) . .  
 H112" H Uiso 0.3480(14) 0.1732(10) -0.0355(11) 1.000 0.057(6) . .  
 H114' H Uiso 0.4218(14) 0.0965(10) 0.1933(10) 1.000 0.051(6) . .  
 H114" H Uiso 0.4129(14) 0.1347(11) 0.1359(10) 1.000 0.059(7) . .  
 H117' H Uiso 0.3756(16) 0.2325(11) 0.3465(10) 1.000 0.062(7) . .  
 H117" H Uiso 0.2902(16) 0.2236(11) 0.3717(11) 1.000 0.064(7) . .  
 H125' H Uiso 0.1763(14) 0.4437(11) 0.2018(10) 1.000 0.058(6) . .  
 H125" H Uiso 0.1030(15) 0.4399(11) 0.2439(10) 1.000 0.056(7) . .  
 H126' H Uiso 0.2953(17) 0.4499(12) 0.2764(11) 1.000 0.075(8) . .  
 H12 H Uiso 0.1019(11) -0.0130(9) 0.0816(8) 1.000 0.034(5) . .  
 H126" H Uiso 0.3025(19) 0.4057(14) 0.3360(13) 1.000 0.093(9) . .  
 H13 H Uiso 0.1377(13) 0.0220(10) -0.0154(9) 1.000 0.050(6) . .  
 H128' H Uiso 0.1655(19) 0.1444(13) 0.4264(12) 1.000 0.088(9) . .  
 H14 H Uiso 0.2228(13) 0.1140(9) -0.0322(9) 1.000 0.046(6) . .  
 H128" H Uiso 0.1125(13) 0.0856(11) 0.4057(9) 1.000 0.048(6) . .  
 H129' H Uiso 0.0001(14) 0.1577(11) 0.2816(11) 1.000 0.058(7) . .  
 H129" H Uiso -0.0349(17) 0.1523(13) 0.3445(12) 1.000 0.077(9) . .  
 H17 H Uiso 0.1289(13) 0.0860(10) 0.2099(9) 1.000 0.052(6) . .

H130' H Uiso 0.0512(14) 0.2770(10) 0.1164(10) 1.000 0.046(6) . .  
H18 H Uiso 0.1902(17) -0.0058(13) 0.2573(13) 1.000 0.086(9) . .  
H18' H Uiso 0.2617(18) 0.0327(14) 0.2176(12) 1.000 0.094(9) . .  
H18" H Uiso 0.1994(16) -0.0348(12) 0.1914(11) 1.000 0.062(8) . .  
H19 H Uiso 0.0049(16) 0.0378(12) 0.1699(11) 1.000 0.073(8) . .  
H19' H Uiso 0.0316(15) 0.0052(11) 0.2320(11) 1.000 0.070(7) . .  
H19" H Uiso 0.0487(17) -0.0322(14) 0.1686(12) 1.000 0.087(9) . .  
H110 H Uiso 0.3094(10) 0.2181(7) 0.0803(8) 1.000 0.023(4) . .  
H111 H Uiso 0.2046(13) 0.2357(10) -0.0235(10) 1.000 0.048(6) . .  
H112 H Uiso 0.4061(14) 0.1563(11) 0.0216(10) 1.000 0.054(6) . .  
H114 H Uiso 0.3581(13) 0.0747(10) 0.1409(9) 1.000 0.044(5) . .  
H115 H Uiso 0.3888(11) 0.1779(8) 0.2603(7) 1.000 0.023(4) . .  
H117 H Uiso 0.3124(15) 0.2857(12) 0.3489(10) 1.000 0.062(7) . .  
H120 H Uiso 0.0984(11) 0.4166(9) 0.3593(8) 1.000 0.037(5) . .  
H121 H Uiso 0.0148(12) 0.3578(9) 0.4252(9) 1.000 0.039(5) . .  
H122 H Uiso 0.0149(13) 0.2415(10) 0.4203(9) 1.000 0.048(6) . .  
H124 H Uiso 0.2373(11) 0.3531(8) 0.2488(8) 1.000 0.029(4) . .  
H125 H Uiso 0.1119(15) 0.3812(11) 0.2017(11) 1.000 0.057(7) . .  
H126 H Uiso 0.2226(16) 0.4626(13) 0.3208(12) 1.000 0.076(8) . .  
H127 H Uiso 0.1411(12) 0.1480(9) 0.3232(8) 1.000 0.034(5) . .  
H128 H Uiso 0.0634(18) 0.1434(13) 0.4351(12) 1.000 0.083(9) . .  
H129 H Uiso 0.0090(15) 0.0923(12) 0.3177(10) 1.000 0.062(7) . .  
H130 H Uiso 0.0044(14) 0.2783(10) 0.1747(10) 1.000 0.053(6) . .  
H132 H Uiso -0.1120(13) 0.2049(10) 0.1960(10) 1.000 0.048(6) . .  
H133 H Uiso -0.2036(14) 0.1186(10) 0.1648(10) 1.000 0.056(6) . .  
H134 H Uiso -0.1734(14) 0.0639(10) 0.0792(10) 1.000 0.053(6) . .  
H135 H Uiso -0.0530(11) 0.0881(9) 0.0262(8) 1.000 0.032(5) . .  
H136 H Uiso 0.0380(12) 0.1728(9) 0.0562(8) 1.000 0.037(5) . .  
H211' H Uiso 0.7555(14) 0.1891(11) 0.0181(10) 1.000 0.057(6) . .  
H211" H Uiso 0.7025(13) 0.2358(10) -0.0216(10) 1.000 0.045(6) . .  
H212' H Uiso 0.8966(14) 0.2472(11) -0.0003(10) 1.000 0.055(6) . .  
H212" H Uiso 0.9050(14) 0.3253(11) 0.0103(10) 1.000 0.054(6) . .  
H22 H Uiso 0.6030(12) 0.5026(9) 0.0322(8) 1.000 0.038(5) . .  
H214' H Uiso 0.9250(14) 0.4146(10) 0.1657(9) 1.000 0.049(6) . .  
H23 H Uiso 0.6334(12) 0.4456(9) -0.0542(9) 1.000 0.043(5) . .  
H214" H Uiso 0.8528(14) 0.4459(11) 0.1294(10) 1.000 0.060(7) . .  
H24 H Uiso 0.7136(10) 0.3505(8) -0.0518(8) 1.000 0.026(4) . .  
H217' H Uiso 0.8830(18) 0.3024(12) 0.3335(11) 1.000 0.074(8) . .  
H217" H Uiso 0.8143(15) 0.2465(12) 0.3429(11) 1.000 0.064(7) . .  
H225' H Uiso 0.7881(15) 0.1274(11) 0.3332(10) 1.000 0.058(7) . .  
H27 H Uiso 0.6758(12) 0.4611(9) 0.1775(8) 1.000 0.032(5) . .  
H225" H Uiso 0.7820(13) 0.0743(10) 0.2814(9) 1.000 0.047(6) . .  
H28 H Uiso 0.518(2) 0.4979(16) 0.1234(15) 1.000 0.113(12) . .  
H28' H Uiso 0.5361(16) 0.4990(12) 0.1933(12) 1.000 0.073(8) . .  
H28" H Uiso 0.5250(16) 0.4342(13) 0.1627(11) 1.000 0.077(8) . .  
H226' H Uiso 0.6564(13) 0.0740(10) 0.2087(9) 1.000 0.044(5) . .  
H29 H Uiso 0.737(3) 0.5516(18) 0.1327(17) 1.000 0.150(16) . .  
H29' H Uiso 0.6644(16) 0.5701(13) 0.1792(12) 1.000 0.080(8) . .  
H29" H Uiso 0.646(2) 0.5689(15) 0.1058(15) 1.000 0.113(12) . .  
H226" H Uiso 0.5936(15) 0.1342(11) 0.2079(10) 1.000 0.060(7) . .  
H228' H Uiso 0.7031(17) 0.3904(12) 0.4083(11) 1.000 0.074(8) . .  
H228" H Uiso 0.6090(15) 0.3978(11) 0.4276(11) 1.000 0.058(7) . .  
H229' H Uiso 0.5024(15) 0.3841(11) 0.2859(12) 1.000 0.063(8) . .  
H229" H Uiso 0.5312(16) 0.4516(13) 0.3123(11) 1.000 0.076(8) . .  
H230' H Uiso 0.5033(12) 0.2369(9) 0.1850(9) 1.000 0.038(5) . .  
H210 H Uiso 0.8041(10) 0.2756(7) 0.0783(8) 1.000 0.023(4) . .  
H211 H Uiso 0.6727(15) 0.2232(10) 0.0457(11) 1.000 0.059(7) . .  
H212 H Uiso 0.8455(14) 0.2930(10) -0.0427(11) 1.000 0.054(6) . .  
H214 H Uiso 0.8974(13) 0.3855(10) 0.1075(10) 1.000 0.053(6) . .  
H215 H Uiso 0.8909(11) 0.3484(8) 0.2441(8) 1.000 0.028(4) . .  
H217 H Uiso 0.7962(17) 0.3097(12) 0.3606(12) 1.000 0.072(8) . .  
H220 H Uiso 0.5740(11) 0.1260(9) 0.3592(8) 1.000 0.033(5) . .  
H221 H Uiso 0.5061(14) 0.1931(10) 0.4235(10) 1.000 0.053(6) . .  
H222 H Uiso 0.5228(11) 0.3057(9) 0.4152(8) 1.000 0.033(5) . .

H224 H Uiso 0.7246(11) 0.1702(8) 0.2466(8) 1.000 0.030(5) . .  
 H225 H Uiso 0.7122(15) 0.0724(11) 0.3343(11) 1.000 0.064(7) . .  
 H226 H Uiso 0.5878(13) 0.0819(10) 0.2589(9) 1.000 0.044(6) . .  
 H227 H Uiso 0.6521(12) 0.3849(9) 0.3092(9) 1.000 0.038(5) . .  
 H228 H Uiso 0.6554(17) 0.4532(13) 0.3925(11) 1.000 0.081(8) . .  
 H229 H Uiso 0.4814(19) 0.3954(14) 0.3489(13) 1.000 0.092(10) . .  
 H230 H Uiso 0.5464(12) 0.2239(9) 0.1240(9) 1.000 0.038(5) . .  
 H232 H Uiso 0.3832(13) 0.3099(9) 0.1887(10) 1.000 0.044(6) . .  
 H233 H Uiso 0.2933(13) 0.3880(10) 0.1430(9) 1.000 0.047(6) . .  
 H234 H Uiso 0.3200(13) 0.4256(10) 0.0482(9) 1.000 0.047(6) . .  
 H235 H Uiso 0.4430(11) 0.3908(9) -0.0007(8) 1.000 0.035(5) . .  
 H236 H Uiso 0.5370(12) 0.3138(9) 0.0449(8) 1.000 0.035(5) . .  
 H31 H Uiso 0.09389 0.49202 0.11254 0.500 0.1031 . .  
 H31' H Uiso 0.18853 0.49830 0.08386 0.500 0.1031 . .  
 H31" H Uiso 0.13096 0.43487 0.07186 0.500 0.1031 . .  
 H32 H Uiso 0.08581 0.56141 0.02836 0.500 0.0547 . .  
 H32' H Uiso 0.12630 0.50590 -0.01265 0.500 0.0547 . .  
 H33 H Uiso -0.03911 0.49579 0.04326 0.500 0.0444 . .  
 H33' H Uiso 0.00107 0.44209 0.00032 0.500 0.0444 . .  
 H34 H Uiso -0.04930 0.56854 -0.03868 0.500 0.0580 . .  
 H34' H Uiso -0.01120 0.51361 -0.08145 0.500 0.0580 . .  
 H35 H Uiso -0.13396 0.44978 -0.06626 0.500 0.1019 . .  
 H35' H Uiso -0.16414 0.51969 -0.08942 0.500 0.1019 . .  
 H35" H Uiso -0.17132 0.50173 -0.02018 0.500 0.1019 . .  
 H41 H Uiso 0.64334 0.07940 0.05247 0.500 0.1400 . .  
 H41' H Uiso 0.66649 0.02000 0.09572 0.500 0.1400 . .  
 H41" H Uiso 0.57592 0.05763 0.10254 0.500 0.1400 . .  
 H42 H Uiso 0.57234 -0.04608 0.05092 0.500 0.0553 . .  
 H42' H Uiso 0.61839 -0.00986 -0.00257 0.500 0.0553 . .  
 H43 H Uiso 0.44354 0.01258 0.03272 0.500 0.0437 . .  
 H43' H Uiso 0.48976 0.05063 -0.02034 0.500 0.0437 . .  
 H44 H Uiso 0.50186 -0.04554 -0.07527 0.500 0.0573 . .  
 H44' H Uiso 0.46190 -0.08606 -0.02155 0.500 0.0573 . .  
 H45 H Uiso 0.33785 -0.03556 -0.03462 0.500 0.1892 . .  
 H45' H Uiso 0.36859 -0.07509 -0.09205 0.500 0.1892 . .  
 H45" H Uiso 0.37853 0.00203 -0.09015 0.500 0.1892 . .

loop\_

\_atom\_site\_aniso\_label  
 \_atom\_site\_aniso\_U\_11  
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 \_atom\_site\_aniso\_U\_23  
 \_atom\_site\_aniso\_U\_13  
 \_atom\_site\_aniso\_U\_12

Fe11 0.0196(1) 0.0243(1) 0.0214(1) -0.0033(1) -0.0020(1) 0.0034(1)  
 N11 0.0189(6) 0.0197(5) 0.0203(6) -0.0004(4) 0.0021(4) -0.0016(4)  
 N12 0.0186(6) 0.0242(6) 0.0187(6) -0.0003(5) 0.0023(4) -0.0009(5)  
 C11 0.0248(8) 0.0206(7) 0.0352(9) -0.0023(6) 0.0006(6) 0.0004(6)  
 C12 0.0349(9) 0.0251(8) 0.0479(11) -0.0109(7) -0.0002(8) -0.0055(7)  
 C13 0.0410(10) 0.0421(10) 0.0413(11) -0.0218(9) 0.0004(8) -0.0081(8)  
 C14 0.0385(10) 0.0466(10) 0.0283(10) -0.0121(8) 0.0060(7) -0.0058(8)  
 C15 0.0267(8) 0.0295(8) 0.0257(8) -0.0057(6) 0.0030(6) -0.0020(6)  
 C16 0.0200(7) 0.0208(7) 0.0259(8) -0.0052(5) 0.0008(6) 0.0023(5)  
 C17 0.0410(10) 0.0272(8) 0.0387(10) 0.0059(7) -0.0002(8) -0.0112(7)  
 C18 0.0490(14) 0.091(2) 0.080(2) 0.0532(18) -0.0117(13) -0.0158(14)  
 C19 0.0362(11) 0.0645(15) 0.0545(14) 0.0137(12) 0.0040(10) -0.0116(10)  
 C110 0.0337(9) 0.0363(9) 0.0228(9) -0.0027(7) 0.0059(7) -0.0095(7)  
 C111 0.0505(12) 0.0425(11) 0.0448(13) 0.0101(9) -0.0006(10) -0.0091(9)  
 C112 0.0420(11) 0.0553(12) 0.0348(11) -0.0046(9) 0.0142(9) -0.0126(10)  
 C113 0.0193(7) 0.0191(6) 0.0237(8) 0.0031(5) 0.0048(5) -0.0010(5)  
 C114 0.0219(8) 0.0275(8) 0.0359(10) -0.0053(7) 0.0023(7) 0.0029(6)  
 C115 0.0155(7) 0.0234(7) 0.0246(8) 0.0033(6) 0.0001(5) -0.0012(5)  
 C116 0.0206(7) 0.0227(7) 0.0207(7) 0.0019(5) 0.0014(5) -0.0037(5)

C117 0.0234(8) 0.0473(10) 0.0243(9) -0.0052(7) -0.0037(7) 0.0020(7)  
C118 0.0184(7) 0.0320(8) 0.0185(7) -0.0026(6) 0.0000(5) 0.0010(6)  
C119 0.0225(7) 0.0314(8) 0.0258(8) -0.0047(6) -0.0003(6) 0.0031(6)  
C120 0.0292(9) 0.0378(9) 0.0330(10) -0.0095(7) -0.0029(7) 0.0093(7)  
C121 0.0264(8) 0.0578(12) 0.0280(9) -0.0094(8) 0.0028(7) 0.0132(8)  
C122 0.0229(8) 0.0564(11) 0.0260(9) 0.0025(8) 0.0059(7) 0.0029(7)  
C123 0.0195(7) 0.0407(9) 0.0228(8) 0.0013(6) 0.0018(6) 0.0001(6)  
C124 0.0340(9) 0.0246(8) 0.0420(10) -0.0035(7) 0.0097(8) 0.0011(7)  
C125 0.0549(13) 0.0523(13) 0.0451(13) 0.0127(10) 0.0135(10) 0.0130(11)  
C126 0.0618(16) 0.0490(14) 0.0776(19) -0.0030(13) 0.0015(14) -0.0225(12)  
C127 0.0331(9) 0.0380(9) 0.0359(10) 0.0043(7) 0.0116(8) -0.0047(7)  
C128 0.0772(18) 0.0437(12) 0.0504(14) 0.0137(10) 0.0075(13) -0.0028(12)  
C129 0.0542(15) 0.0549(15) 0.083(2) -0.0080(14) -0.0114(14) -0.0142(12)  
C130 0.0282(9) 0.0333(9) 0.0364(10) -0.0071(8) -0.0076(7) 0.0078(7)  
C131 0.0254(8) 0.0356(8) 0.0300(9) -0.0038(7) -0.0066(6) 0.0096(6)  
C132 0.0316(9) 0.0459(10) 0.0343(10) -0.0130(8) 0.0029(7) 0.0078(8)  
C133 0.0303(10) 0.0526(12) 0.0498(12) -0.0138(9) 0.0122(9) -0.0010(8)  
C134 0.0306(9) 0.0472(11) 0.0509(12) -0.0194(9) 0.0033(8) -0.0033(8)  
C135 0.0320(9) 0.0471(10) 0.0341(10) -0.0154(8) 0.0017(7) 0.0032(8)  
C136 0.0260(8) 0.0431(10) 0.0288(9) -0.0047(7) -0.0018(7) 0.0039(7)  
Fe21 0.0199(1) 0.0281(1) 0.0180(1) 0.0037(1) -0.0006(1) -0.0040(1)  
N21 0.0223(6) 0.0245(6) 0.0170(6) -0.0006(5) 0.0031(5) -0.0012(5)  
N22 0.0195(6) 0.0287(6) 0.0166(6) 0.0011(5) 0.0028(4) 0.0017(5)  
C21 0.0286(8) 0.0218(7) 0.0250(8) -0.0010(6) 0.0038(6) -0.0039(6)  
C22 0.0383(9) 0.0236(8) 0.0322(9) 0.0044(6) 0.0012(7) 0.0009(7)  
C23 0.0415(10) 0.0345(9) 0.0224(9) 0.0069(7) 0.0003(7) 0.0003(7)  
C24 0.0354(9) 0.0342(8) 0.0194(8) -0.0010(6) 0.0042(6) -0.0010(7)  
C25 0.0243(7) 0.0256(7) 0.0213(8) 0.0004(6) 0.0040(6) -0.0029(6)  
C26 0.0218(7) 0.0230(7) 0.0191(7) 0.0012(5) 0.0024(5) -0.0052(5)  
C27 0.0433(10) 0.0278(8) 0.0266(9) -0.0042(7) 0.0000(7) 0.0033(7)  
C28 0.0529(14) 0.0738(17) 0.0561(16) -0.0308(14) 0.0189(12) -0.0014(12)  
C29 0.118(3) 0.0378(12) 0.0644(18) -0.0239(12) 0.0180(18) -0.0235(14)  
C210 0.0305(8) 0.0324(8) 0.0218(8) -0.0029(6) 0.0049(6) 0.0042(6)  
C211 0.0466(12) 0.0295(9) 0.0614(15) -0.0094(9) 0.0000(10) 0.0042(8)  
C212 0.0381(10) 0.0537(12) 0.0331(11) -0.0003(9) 0.0129(8) 0.0115(9)  
C213 0.0213(7) 0.0239(7) 0.0226(8) -0.0046(6) 0.0055(5) -0.0008(5)  
C214 0.0238(8) 0.0385(9) 0.0283(9) -0.0014(7) 0.0039(7) -0.0089(7)  
C215 0.0163(7) 0.0332(8) 0.0226(8) -0.0050(6) 0.0012(6) -0.0007(6)  
C216 0.0224(7) 0.0290(7) 0.0195(8) -0.0033(6) 0.0003(6) 0.0057(6)  
C217 0.0261(9) 0.0536(12) 0.0245(9) 0.0037(8) -0.0040(7) 0.0014(8)  
C218 0.0181(7) 0.0353(8) 0.0153(7) 0.0027(6) -0.0001(5) 0.0021(6)  
C219 0.0201(7) 0.0365(8) 0.0196(8) 0.0050(6) -0.0009(6) 0.0016(6)  
C220 0.0262(8) 0.0401(10) 0.0277(9) 0.0114(7) -0.0007(6) -0.0026(7)  
C221 0.0224(8) 0.0579(11) 0.0247(9) 0.0122(8) 0.0056(6) 0.0006(7)  
C222 0.0253(8) 0.0514(10) 0.0233(9) 0.0024(7) 0.0067(6) 0.0088(7)  
C223 0.0241(8) 0.0415(9) 0.0198(8) 0.0011(6) 0.0027(6) 0.0050(6)  
C224 0.0296(8) 0.0297(8) 0.0257(9) 0.0037(6) 0.0030(6) 0.0000(6)  
C225 0.0431(12) 0.0563(13) 0.0416(12) -0.0018(10) -0.0047(9) 0.0202(10)  
C226 0.0430(11) 0.0399(10) 0.0454(12) -0.0050(9) -0.0049(9) 0.0012(9)  
C227 0.0425(10) 0.0400(10) 0.0315(10) -0.0015(8) 0.0149(8) 0.0082(8)  
C228 0.0741(17) 0.0447(12) 0.0460(13) -0.0137(10) 0.0095(12) 0.0052(12)  
C229 0.0706(18) 0.0522(14) 0.0728(19) 0.0131(14) -0.0019(15) 0.0219(13)  
C230 0.0272(8) 0.0312(8) 0.0299(9) 0.0066(7) -0.0031(7) -0.0066(7)  
C231 0.0249(8) 0.0263(8) 0.0292(9) 0.0018(6) -0.0008(6) -0.0077(6)  
C232 0.0322(9) 0.0386(9) 0.0349(10) 0.0082(8) 0.0094(7) -0.0039(7)  
C233 0.0343(10) 0.0433(10) 0.0511(12) 0.0060(9) 0.0154(9) 0.0061(8)  
C234 0.0344(9) 0.0361(9) 0.0474(12) 0.0105(8) 0.0027(8) 0.0063(7)  
C235 0.0349(9) 0.0357(9) 0.0299(9) 0.0082(7) 0.0014(7) -0.0002(7)  
C236 0.0256(8) 0.0304(8) 0.0279(9) 0.0005(6) 0.0010(6) -0.0009(6)  
C31 0.060(4) 0.092(5) 0.053(4) 0.017(3) -0.006(3) 0.011(4)  
C32 0.051(2) 0.044(2) 0.042(2) -0.0008(18) 0.007(2) -0.0045(19)  
C33 0.042(2) 0.032(4) 0.037(4) 0.002(2) 0.014(2) 0.003(3)  
C34 0.045(2) 0.057(3) 0.043(2) 0.008(2) 0.010(2) -0.002(2)  
C35 0.045(3) 0.100(6) 0.059(5) 0.015(3) -0.009(3) -0.004(3)

C41 0.139(11) 0.066(5) 0.073(8) 0.016(4) -0.034(6) -0.031(5)  
 C42 0.038(2) 0.062(3) 0.039(2) 0.0121(19) 0.0014(17) -0.0011(19)  
 C43 0.034(4) 0.038(4) 0.0372(19) 0.008(3) 0.012(3) 0.007(2)  
 C44 0.037(2) 0.069(3) 0.038(2) -0.0005(19) 0.0090(17) 0.009(2)  
 C45 0.112(9) 0.234(15) 0.032(4) 0.007(6) -0.016(4) -0.102(9)

#=====

# # 10. MOLECULAR GEOMETRY

\_geom\_special\_details

;  
 Bond distances, angles etc. have been calculated using the  
 rounded fractional coordinates. All esds are estimated  
 from the variances of the (full) variance-covariance matrix.  
 The cell esds are taken into account in the estimation of  
 distances, angles and torsion angles  
 ;

loop\_

\_geom\_bond\_atom\_site\_label\_1  
 \_geom\_bond\_atom\_site\_label\_2  
 \_geom\_bond\_distance  
 \_geom\_bond\_site\_symmetry\_1  
 \_geom\_bond\_site\_symmetry\_2  
 \_geom\_bond\_publ\_flag

Fe11	N11	1.9831(11)	.	.	yes
Fe11	N12	1.9807(11)	.	.	yes
Fe11	C130	2.0414(18)	.	.	yes
Fe21	N22	1.9773(12)	.	.	yes
Fe21	C230	2.0404(17)	.	.	yes
Fe21	N21	1.9803(12)	.	.	yes
N11	C16	1.4426(19)	.	.	yes
N11	C113	1.3321(17)	.	.	yes
N12	C116	1.3405(18)	.	.	yes
N12	C118	1.4423(19)	.	.	yes
N21	C26	1.4432(18)	.	.	yes
N21	C213	1.3341(19)	.	.	yes
N22	C218	1.4415(18)	.	.	yes
N22	C216	1.3342(19)	.	.	yes
C11	C12	1.395(2)	.	.	no
C11	C16	1.413(2)	.	.	no
C11	C17	1.514(2)	.	.	no
C12	C13	1.382(3)	.	.	no
C13	C14	1.379(3)	.	.	no
C14	C15	1.399(2)	.	.	no
C15	C16	1.402(2)	.	.	no
C15	C110	1.520(2)	.	.	no
C17	C18	1.514(4)	.	.	no
C17	C19	1.521(3)	.	.	no
C110	C112	1.536(3)	.	.	no
C110	C111	1.533(3)	.	.	no
C12	H12	1.012(18)	.	.	no
C113	C114	1.512(2)	.	.	no
C113	C115	1.405(2)	.	.	no
C13	H13	0.92(2)	.	.	no
C14	H14	0.95(2)	.	.	no
C115	C116	1.401(2)	.	.	no
C116	C117	1.504(2)	.	.	no
C17	H17	1.00(2)	.	.	no
C18	H18"	1.00(2)	.	.	no
C18	H18	0.97(3)	.	.	no
C18	H18'	1.04(3)	.	.	no
C118	C119	1.406(2)	.	.	no

C118	C123	1.408(2)	.	.	no
C119	C120	1.396(2)	.	.	no
C119	C124	1.517(2)	.	.	no
C19	H19	0.94(2)	.	.	no
C19	H19'	1.01(2)	.	.	no
C19	H19"	1.03(3)	.	.	no
C120	C121	1.386(3)	.	.	no
C121	C122	1.372(3)	.	.	no
C122	C123	1.400(2)	.	.	no
C123	C127	1.521(2)	.	.	no
C124	C125	1.523(3)	.	.	no
C124	C126	1.536(3)	.	.	no
C127	C128	1.524(3)	.	.	no
C127	C129	1.521(3)	.	.	no
C130	C131	1.487(2)	.	.	no
C131	C132	1.400(2)	.	.	no
C131	C136	1.403(3)	.	.	no
C132	C133	1.383(3)	.	.	no
C133	C134	1.381(3)	.	.	no
C134	C135	1.386(3)	.	.	no
C135	C136	1.384(3)	.	.	no
C110	H110	0.973(17)	.	.	no
C111	H111'	0.94(2)	.	.	no
C111	H111"	1.03(2)	.	.	no
C111	H111	0.97(2)	.	.	no
C112	H112'	0.98(2)	.	.	no
C112	H112"	0.96(2)	.	.	no
C112	H112	0.98(2)	.	.	no
C114	H114"	0.93(2)	.	.	no
C114	H114	0.97(2)	.	.	no
C114	H114'	0.95(2)	.	.	no
C115	H115	0.912(17)	.	.	no
C117	H117	0.94(2)	.	.	no
C117	H117"	0.89(2)	.	.	no
C117	H117'	0.89(2)	.	.	no
C120	H120	0.947(19)	.	.	no
C121	H121	0.950(19)	.	.	no
C21	C27	1.522(2)	.	.	no
C21	C26	1.410(2)	.	.	no
C21	C22	1.389(2)	.	.	no
C122	H122	0.97(2)	.	.	no
C22	C23	1.380(2)	.	.	no
C23	C24	1.385(2)	.	.	no
C24	C25	1.389(2)	.	.	no
C124	H124	0.956(17)	.	.	no
C25	C26	1.407(2)	.	.	no
C125	H125"	0.88(2)	.	.	no
C125	H125	1.00(2)	.	.	no
C125	H125'	0.97(2)	.	.	no
C25	C210	1.523(2)	.	.	no
C126	H126'	0.93(3)	.	.	no
C126	H126"	1.08(3)	.	.	no
C126	H126	0.96(3)	.	.	no
C27	C28	1.513(3)	.	.	no
C127	H127	0.952(18)	.	.	no
C27	C29	1.531(3)	.	.	no
C128	H128"	0.94(2)	.	.	no
C128	H128	0.97(3)	.	.	no
C128	H128'	0.97(3)	.	.	no
C129	H129	0.96(2)	.	.	no
C129	H129'	0.97(2)	.	.	no
C129	H129"	0.92(3)	.	.	no
C130	H130	0.90(2)	.	.	no
C130	H130'	0.93(2)	.	.	no

C132	H132	0.93(2)	.	.	no
C133	H133	0.93(2)	.	.	no
C134	H134	0.91(2)	.	.	no
C135	H135	0.917(18)	.	.	no
C136	H136	0.916(18)	.	.	no
C22	H22	0.970(19)	.	.	no
C23	H23	0.94(2)	.	.	no
C24	H24	0.963(18)	.	.	no
C27	H27	0.917(18)	.	.	no
C28	H28'	0.92(3)	.	.	no
C28	H28"	0.96(3)	.	.	no
C28	H28	1.00(3)	.	.	no
C29	H29'	0.98(3)	.	.	no
C29	H29	0.96(5)	.	.	no
C29	H29"	1.01(3)	.	.	no
C210	C211	1.536(3)	.	.	no
C210	C212	1.534(3)	.	.	no
C213	C214	1.509(2)	.	.	no
C213	C215	1.404(2)	.	.	no
C215	C216	1.404(2)	.	.	no
C216	C217	1.511(2)	.	.	no
C218	C219	1.405(2)	.	.	no
C218	C223	1.410(2)	.	.	no
C219	C220	1.397(2)	.	.	no
C219	C224	1.519(2)	.	.	no
C220	C221	1.384(2)	.	.	no
C221	C222	1.377(3)	.	.	no
C222	C223	1.398(2)	.	.	no
C223	C227	1.521(2)	.	.	no
C224	C225	1.536(3)	.	.	no
C224	C226	1.527(3)	.	.	no
C227	C228	1.527(3)	.	.	no
C227	C229	1.522(4)	.	.	no
C230	C231	1.491(2)	.	.	no
C31	C32	1.537(8)	.	.	no
C231	C236	1.401(2)	.	.	no
C231	C232	1.403(2)	.	.	no
C32	C33	1.511(9)	.	.	no
C232	C233	1.384(3)	.	.	no
C33	C34	1.515(8)	.	.	no
C233	C234	1.386(3)	.	.	no
C34	C35	1.496(8)	.	.	no
C234	C235	1.386(3)	.	.	no
C235	C236	1.384(2)	.	.	no
C210	H210	0.955(18)	.	.	no
C211	H211'	0.94(2)	.	.	no
C211	H211"	1.00(2)	.	.	no
C211	H211	0.98(2)	.	.	no
C212	H212"	1.04(2)	.	.	no
C212	H212	0.96(2)	.	.	no
C212	H212'	0.99(2)	.	.	no
C214	H214	0.92(2)	.	.	no
C214	H214'	0.91(2)	.	.	no
C214	H214"	0.99(2)	.	.	no
C215	H215	0.915(17)	.	.	no
C217	H217"	0.97(2)	.	.	no
C217	H217	0.88(3)	.	.	no
C217	H217'	0.91(3)	.	.	no
C220	H220	0.915(19)	.	.	no
C221	H221	0.93(2)	.	.	no
C222	H222	0.951(18)	.	.	no
C224	H224	0.961(17)	.	.	no
C225	H225'	0.97(2)	.	.	no
C225	H225	0.99(2)	.	.	no

C225	H225"	0.99(2)	.	.	no
C226	H226'	1.00(2)	.	.	no
C226	H226"	0.96(2)	.	.	no
C226	H226	0.93(2)	.	.	no
C227	H227	0.927(19)	.	.	no
C228	H228	0.95(3)	.	.	no
C228	H228'	0.96(3)	.	.	no
C228	H228"	0.95(2)	.	.	no
C229	H229"	0.96(3)	.	.	no
C229	H229	0.95(3)	.	.	no
C229	H229'	0.97(3)	.	.	no
C230	H230'	0.96(2)	.	.	no
C230	H230	0.942(19)	.	.	no
C31	H31"	0.9802	.	.	no
C31	H31	0.9796	.	.	no
C31	H31'	0.9804	.	.	no
C232	H232	0.94(2)	.	.	no
C32	H32	0.9904	.	.	no
C32	H32'	0.9900	.	.	no
C233	H233	0.90(2)	.	.	no
C33	H33	0.9900	.	.	no
C33	H33'	0.9908	.	.	no
C34	H34'	0.9896	.	.	no
C234	H234	0.94(2)	.	.	no
C34	H34	0.9905	.	.	no
C35	H35'	0.9795	.	.	no
C235	H235	0.959(18)	.	.	no
C35	H35	0.9794	.	.	no
C35	H35"	0.9805	.	.	no
C236	H236	0.964(18)	.	.	no
C41	C42	1.511(15)	.	.	no
C42	C43	1.528(9)	.	.	no
C43	C44	1.524(9)	.	.	no
C44	C45	1.309(16)	.	.	no
C41	H41	0.9790	.	.	no
C41	H41'	0.9800	.	.	no
C41	H41"	0.9803	.	.	no
C42	H42	0.9905	.	.	no
C42	H42'	0.9899	.	.	no
C43	H43	0.9898	.	.	no
C43	H43'	0.9892	.	.	no
C44	H44	0.9906	.	.	no
C44	H44'	0.9905	.	.	no
C45	H45	0.9790	.	.	no
C45	H45'	0.9813	.	.	no
C45	H45"	0.9797	.	.	no

loop\_

\_geom\_angle\_atom\_site\_label\_1

\_geom\_angle\_atom\_site\_label\_2

\_geom\_angle\_atom\_site\_label\_3

\_geom\_angle

\_geom\_angle\_site\_symmetry\_1

\_geom\_angle\_site\_symmetry\_2

\_geom\_angle\_site\_symmetry\_3

\_geom\_angle\_publ\_flag

N11	Fe11	N12	94.35(5)	.	.	.	yes
N11	Fe11	C130	131.81(6)	.	.	.	yes
N12	Fe11	C130	133.84(6)	.	.	.	yes
N22	Fe21	C230	130.28(6)	.	.	.	yes
N21	Fe21	N22	94.15(5)	.	.	.	yes
N21	Fe21	C230	135.51(6)	.	.	.	yes
Fe11	N11	C16	115.54(8)	.	.	.	yes
C16	N11	C113	120.05(11)	.	.	.	yes



Fe11	N11	C113	124.38(9)	.	.	.	yes
C116	N12	C118	118.32(12)	.	.	.	yes
Fe11	N12	C116	123.69(10)	.	.	.	yes
Fe11	N12	C118	117.97(9)	.	.	.	yes
C26	N21	C213	120.68(12)	.	.	.	yes
Fe21	N21	C213	124.54(10)	.	.	.	yes
Fe21	N21	C26	114.77(9)	.	.	.	yes
Fe21	N22	C218	115.42(9)	.	.	.	yes
C216	N22	C218	120.01(12)	.	.	.	yes
Fe21	N22	C216	124.48(10)	.	.	.	yes
C12	C11	C16	117.72(15)	.	.	.	no
C12	C11	C17	121.26(14)	.	.	.	no
C16	C11	C17	121.03(14)	.	.	.	no
C11	C12	C13	121.10(16)	.	.	.	no
C12	C13	C14	120.39(17)	.	.	.	no
C13	C14	C15	121.07(17)	.	.	.	no
C14	C15	C110	119.51(15)	.	.	.	no
C14	C15	C16	117.94(14)	.	.	.	no
C16	C15	C110	122.50(14)	.	.	.	no
N11	C16	C15	120.49(12)	.	.	.	yes
N11	C16	C11	117.57(13)	.	.	.	yes
C11	C16	C15	121.75(14)	.	.	.	no
C11	C17	C19	113.86(16)	.	.	.	no
C18	C17	C19	109.95(19)	.	.	.	no
C11	C17	C18	111.98(17)	.	.	.	no
C15	C110	C112	112.26(15)	.	.	.	no
C111	C110	C112	110.36(16)	.	.	.	no
C15	C110	C111	110.23(14)	.	.	.	no
C11	C12	H12	117.4(10)	.	.	.	no
C13	C12	H12	121.5(10)	.	.	.	no
C114	C113	C115	116.92(13)	.	.	.	no
C12	C13	H13	119.2(13)	.	.	.	no
C14	C13	H13	120.4(13)	.	.	.	no
N11	C113	C114	119.96(12)	.	.	.	yes
N11	C113	C115	123.12(12)	.	.	.	yes
C13	C14	H14	121.0(12)	.	.	.	no
C15	C14	H14	117.9(12)	.	.	.	no
C113	C115	C116	128.97(13)	.	.	.	no
N12	C116	C117	119.34(14)	.	.	.	yes
N12	C116	C115	123.76(14)	.	.	.	yes
C115	C116	C117	116.89(13)	.	.	.	no
C11	C17	H17	108.8(12)	.	.	.	no
C18	C17	H17	107.7(12)	.	.	.	no
C19	C17	H17	104.0(12)	.	.	.	no
H18	C18	H18"	109(2)	.	.	.	no
N12	C118	C119	119.87(13)	.	.	.	yes
H18'	C18	H18"	123(2)	.	.	.	no
C17	C18	H18	112.1(16)	.	.	.	no
C17	C18	H18'	106.1(16)	.	.	.	no
C17	C18	H18"	98.2(14)	.	.	.	no
H18	C18	H18'	108(2)	.	.	.	no
N12	C118	C123	119.08(13)	.	.	.	yes
C119	C118	C123	121.01(14)	.	.	.	no
C17	C19	H19'	110.3(13)	.	.	.	no
C17	C19	H19	110.3(15)	.	.	.	no
C120	C119	C124	119.54(14)	.	.	.	no
H19	C19	H19"	108(2)	.	.	.	no
H19'	C19	H19"	107(2)	.	.	.	no
C17	C19	H19"	112.1(15)	.	.	.	no
H19	C19	H19'	109(2)	.	.	.	no
C118	C119	C120	118.49(14)	.	.	.	no
C118	C119	C124	121.96(14)	.	.	.	no
C119	C120	C121	120.94(17)	.	.	.	no
C120	C121	C122	120.03(17)	.	.	.	no

C121	C122	C123	121.50(17)	.	.	.	no
C122	C123	C127	120.14(15)	.	.	.	no
C118	C123	C122	118.03(15)	.	.	.	no
C118	C123	C127	121.82(14)	.	.	.	no
C125	C124	C126	111.12(17)	.	.	.	no
C119	C124	C126	112.13(17)	.	.	.	no
C119	C124	C125	110.76(15)	.	.	.	no
C123	C127	C129	110.90(17)	.	.	.	no
C123	C127	C128	112.42(16)	.	.	.	no
C128	C127	C129	110.3(2)	.	.	.	no
Fe11	C130	C131	113.18(11)	.	.	.	yes
C132	C131	C136	116.74(15)	.	.	.	no
C130	C131	C132	121.59(16)	.	.	.	no
C130	C131	C136	121.66(15)	.	.	.	no
C131	C132	C133	121.59(17)	.	.	.	no
C132	C133	C134	120.82(18)	.	.	.	no
C133	C134	C135	118.65(18)	.	.	.	no
C134	C135	C136	120.78(17)	.	.	.	no
C131	C136	C135	121.41(16)	.	.	.	no
C111	C110	H110	107.8(9)	.	.	.	no
C15	C110	H110	108.8(9)	.	.	.	no
C112	C110	H110	107.2(9)	.	.	.	no
C110	C111	H111"	111.9(11)	.	.	.	no
C110	C111	H111	109.2(12)	.	.	.	no
C110	C111	H111'	110.3(12)	.	.	.	no
H111'	C111	H111	106.3(18)	.	.	.	no
H111"	C111	H111	108.7(17)	.	.	.	no
H111'	C111	H111"	110.3(16)	.	.	.	no
C110	C112	H112	110.9(13)	.	.	.	no
H112'	C112	H112"	110.3(18)	.	.	.	no
H112'	C112	H112	106.2(18)	.	.	.	no
H112"	C112	H112	109.9(18)	.	.	.	no
C110	C112	H112"	110.3(13)	.	.	.	no
C110	C112	H112'	109.2(12)	.	.	.	no
C113	C114	H114"	109.3(14)	.	.	.	no
C113	C114	H114'	110.7(13)	.	.	.	no
H114'	C114	H114	110.9(18)	.	.	.	no
C113	C114	H114	113.6(12)	.	.	.	no
H114'	C114	H114"	107.7(19)	.	.	.	no
H114"	C114	H114	104.3(18)	.	.	.	no
C116	C115	H115	113.2(10)	.	.	.	no
C113	C115	H115	117.6(10)	.	.	.	no
H117'	C117	H117"	109(2)	.	.	.	no
C116	C117	H117'	114.9(14)	.	.	.	no
H117'	C117	H117	106(2)	.	.	.	no
H117"	C117	H117	102(2)	.	.	.	no
C116	C117	H117	111.7(14)	.	.	.	no
C116	C117	H117"	112.3(16)	.	.	.	no
C121	C120	H120	120.8(11)	.	.	.	no
C119	C120	H120	118.3(11)	.	.	.	no
C22	C21	C26	118.28(14)	.	.	.	no
C120	C121	H121	117.8(11)	.	.	.	no
C122	C121	H121	122.2(11)	.	.	.	no
C22	C21	C27	119.30(14)	.	.	.	no
C26	C21	C27	122.42(14)	.	.	.	no
C121	C122	H122	122.8(12)	.	.	.	no
C21	C22	C23	121.28(15)	.	.	.	no
C123	C122	H122	115.6(12)	.	.	.	no
C22	C23	C24	119.78(16)	.	.	.	no
C23	C24	C25	121.46(15)	.	.	.	no
C119	C124	H124	108.5(10)	.	.	.	no
C125	C124	H124	105.5(11)	.	.	.	no
C126	C124	H124	108.5(10)	.	.	.	no
C124	C125	H125'	109.4(13)	.	.	.	no

C124	C125	H125"	112.0(15)	.	.	.	no
C124	C125	H125	108.3(14)	.	.	.	no
H125'	C125	H125"	106(2)	.	.	.	no
H125'	C125	H125	111.0(19)	.	.	.	no
H125"	C125	H125	110(2)	.	.	.	no
C26	C25	C210	122.39(13)	.	.	.	no
C24	C25	C26	118.07(13)	.	.	.	no
C24	C25	C210	119.52(14)	.	.	.	no
C124	C126	H126"	110.5(16)	.	.	.	no
H126'	C126	H126	108(2)	.	.	.	no
C124	C126	H126	106.9(15)	.	.	.	no
H126'	C126	H126"	107(2)	.	.	.	no
C124	C126	H126'	107.7(16)	.	.	.	no
N21	C26	C21	118.96(12)	.	.	.	yes
N21	C26	C25	119.73(13)	.	.	.	yes
C21	C26	C25	121.10(13)	.	.	.	no
H126"	C126	H126	116(2)	.	.	.	no
C21	C27	C29	111.04(18)	.	.	.	no
C28	C27	C29	109.5(2)	.	.	.	no
C21	C27	C28	111.65(17)	.	.	.	no
C123	C127	H127	108.1(11)	.	.	.	no
C128	C127	H127	107.1(11)	.	.	.	no
C129	C127	H127	107.8(11)	.	.	.	no
C127	C128	H128'	110.9(16)	.	.	.	no
C127	C128	H128"	110.8(13)	.	.	.	no
C127	C128	H128	108.6(16)	.	.	.	no
H128'	C128	H128	109(2)	.	.	.	no
H128"	C128	H128	110(2)	.	.	.	no
H128'	C128	H128"	107(2)	.	.	.	no
C127	C129	H129'	110.7(13)	.	.	.	no
C127	C129	H129"	108.1(17)	.	.	.	no
H129'	C129	H129"	107(2)	.	.	.	no
H129'	C129	H129	109.9(19)	.	.	.	no
C127	C129	H129	110.7(14)	.	.	.	no
H129"	C129	H129	110(2)	.	.	.	no
Fe11	C130	H130'	103.3(13)	.	.	.	no
Fe11	C130	H130	106.1(14)	.	.	.	no
C131	C130	H130'	113.1(13)	.	.	.	no
C131	C130	H130	111.3(14)	.	.	.	no
H130'	C130	H130	109.4(19)	.	.	.	no
C131	C132	H132	117.2(13)	.	.	.	no
C133	C132	H132	121.2(12)	.	.	.	no
C132	C133	H133	122.8(13)	.	.	.	no
C134	C133	H133	116.3(13)	.	.	.	no
C135	C134	H134	118.8(14)	.	.	.	no
C133	C134	H134	122.3(14)	.	.	.	no
C134	C135	H135	118.6(11)	.	.	.	no
C136	C135	H135	120.6(11)	.	.	.	no
C135	C136	H136	121.5(12)	.	.	.	no
C131	C136	H136	117.0(12)	.	.	.	no
C23	C22	H22	118.4(11)	.	.	.	no
C21	C22	H22	120.3(11)	.	.	.	no
C22	C23	H23	120.6(12)	.	.	.	no
C24	C23	H23	119.6(12)	.	.	.	no
C25	C24	H24	119.4(10)	.	.	.	no
C23	C24	H24	119.1(10)	.	.	.	no
C21	C27	H27	109.1(12)	.	.	.	no
C29	C27	H27	103.9(12)	.	.	.	no
C28	C27	H27	111.4(11)	.	.	.	no
C27	C28	H28'	110.5(16)	.	.	.	no
C27	C28	H28"	112.3(15)	.	.	.	no
H28	C28	H28"	108(2)	.	.	.	no
H28'	C28	H28"	107(2)	.	.	.	no
H28	C28	H28'	112(2)	.	.	.	no

C27	C28	H28	106.6(18)	.	.	.	no
C27	C29	H29'	108.8(15)	.	.	.	no
C27	C29	H29"	108.5(18)	.	.	.	no
H29	C29	H29'	109(3)	.	.	.	no
H29	C29	H29"	104(3)	.	.	.	no
H29'	C29	H29"	113(2)	.	.	.	no
C27	C29	H29	114(2)	.	.	.	no
C25	C210	C212	111.72(14)	.	.	.	no
C25	C210	C211	110.30(14)	.	.	.	no
C211	C210	C212	110.51(16)	.	.	.	no
C214	C213	C215	117.31(13)	.	.	.	no
N21	C213	C214	119.33(14)	.	.	.	yes
N21	C213	C215	123.36(13)	.	.	.	yes
C213	C215	C216	128.76(13)	.	.	.	no
N22	C216	C215	123.48(14)	.	.	.	yes
N22	C216	C217	119.79(14)	.	.	.	yes
C215	C216	C217	116.73(13)	.	.	.	no
C219	C218	C223	121.15(13)	.	.	.	no
N22	C218	C223	118.77(13)	.	.	.	yes
N22	C218	C219	119.93(12)	.	.	.	yes
C218	C219	C220	118.13(14)	.	.	.	no
C220	C219	C224	119.78(15)	.	.	.	no
C218	C219	C224	122.10(13)	.	.	.	no
C219	C220	C221	121.38(17)	.	.	.	no
C220	C221	C222	119.80(16)	.	.	.	no
C221	C222	C223	121.39(16)	.	.	.	no
C218	C223	C227	122.34(14)	.	.	.	no
C218	C223	C222	118.12(15)	.	.	.	no
C222	C223	C227	119.52(15)	.	.	.	no
C219	C224	C225	111.69(14)	.	.	.	no
C219	C224	C226	111.77(14)	.	.	.	no
C225	C224	C226	110.07(16)	.	.	.	no
C223	C227	C229	111.07(17)	.	.	.	no
C228	C227	C229	110.4(2)	.	.	.	no
C223	C227	C228	111.93(16)	.	.	.	no
Fe21	C230	C231	113.41(11)	.	.	.	yes
C230	C231	C232	121.68(15)	.	.	.	no
C230	C231	C236	121.40(14)	.	.	.	no
C232	C231	C236	116.91(14)	.	.	.	no
C231	C232	C233	121.35(17)	.	.	.	no
C31	C32	C33	112.8(5)	.	.	.	no
C232	C233	C234	120.79(18)	.	.	.	no
C32	C33	C34	114.8(5)	.	.	.	no
C233	C234	C235	118.74(17)	.	.	.	no
C33	C34	C35	112.3(5)	.	.	.	no
C234	C235	C236	120.66(16)	.	.	.	no
C231	C236	C235	121.54(15)	.	.	.	no
C25	C210	H210	109.3(9)	.	.	.	no
C211	C210	H210	107.5(9)	.	.	.	no
C212	C210	H210	107.4(9)	.	.	.	no
C210	C211	H211	113.0(13)	.	.	.	no
H211'	C211	H211"	105.0(18)	.	.	.	no
H211"	C211	H211	108.4(18)	.	.	.	no
C210	C211	H211"	108.5(12)	.	.	.	no
H211'	C211	H211	111.1(18)	.	.	.	no
C210	C211	H211'	110.6(13)	.	.	.	no
C210	C212	H212'	111.1(13)	.	.	.	no
H212'	C212	H212	105.3(18)	.	.	.	no
H212"	C212	H212	109.4(18)	.	.	.	no
C210	C212	H212	111.0(13)	.	.	.	no
H212'	C212	H212"	107.5(18)	.	.	.	no
C210	C212	H212"	112.2(12)	.	.	.	no
C213	C214	H214'	112.9(13)	.	.	.	no
C213	C214	H214"	110.9(13)	.	.	.	no

H214"	C214	H214	104.2(19)	.	.	.	no
H214'	C214	H214	109.1(18)	.	.	.	no
H214'	C214	H214"	105.7(18)	.	.	.	no
C213	C214	H214	113.3(13)	.	.	.	no
C213	C215	H215	116.6(11)	.	.	.	no
C216	C215	H215	114.6(11)	.	.	.	no
C216	C217	H217'	112.1(16)	.	.	.	no
C216	C217	H217"	110.0(14)	.	.	.	no
C216	C217	H217	110.4(17)	.	.	.	no
H217'	C217	H217"	114(2)	.	.	.	no
H217'	C217	H217	111(2)	.	.	.	no
H217"	C217	H217	98(2)	.	.	.	no
C221	C220	H220	118.9(11)	.	.	.	no
C219	C220	H220	119.7(11)	.	.	.	no
C220	C221	H221	118.1(13)	.	.	.	no
C222	C221	H221	122.0(13)	.	.	.	no
C221	C222	H222	120.2(11)	.	.	.	no
C223	C222	H222	118.4(11)	.	.	.	no
C226	C224	H224	108.5(11)	.	.	.	no
C225	C224	H224	106.2(10)	.	.	.	no
C219	C224	H224	108.4(10)	.	.	.	no
C224	C225	H225'	109.5(13)	.	.	.	no
C224	C225	H225"	108.8(12)	.	.	.	no
C224	C225	H225	108.9(14)	.	.	.	no
H225'	C225	H225"	109.4(18)	.	.	.	no
H225'	C225	H225	111.6(19)	.	.	.	no
H225"	C225	H225	108.6(18)	.	.	.	no
C224	C226	H226"	108.3(14)	.	.	.	no
H226'	C226	H226	107.7(17)	.	.	.	no
C224	C226	H226	109.8(13)	.	.	.	no
H226'	C226	H226"	106.7(18)	.	.	.	no
C224	C226	H226'	112.0(12)	.	.	.	no
H226"	C226	H226	112.4(19)	.	.	.	no
C228	C227	H227	107.1(12)	.	.	.	no
C229	C227	H227	108.7(12)	.	.	.	no
C223	C227	H227	107.4(12)	.	.	.	no
C227	C228	H228"	108.3(14)	.	.	.	no
H228'	C228	H228	106(2)	.	.	.	no
C227	C228	H228	113.2(15)	.	.	.	no
H228'	C228	H228"	105(2)	.	.	.	no
C227	C228	H228'	112.3(15)	.	.	.	no
H228"	C228	H228	111(2)	.	.	.	no
C227	C229	H229	110.9(18)	.	.	.	no
H229'	C229	H229	100(2)	.	.	.	no
H229"	C229	H229	116(2)	.	.	.	no
H229'	C229	H229"	109(2)	.	.	.	no
C227	C229	H229'	109.1(14)	.	.	.	no
C227	C229	H229"	110.8(15)	.	.	.	no
C231	C230	H230	111.9(12)	.	.	.	no
H230'	C230	H230	109.4(16)	.	.	.	no
Fe21	C230	H230'	104.9(11)	.	.	.	no
Fe21	C230	H230	105.2(11)	.	.	.	no
C231	C230	H230'	111.6(11)	.	.	.	no
C32	C31	H31"	109.47	.	.	.	no
H31	C31	H31'	109.46	.	.	.	no
H31	C31	H31"	109.49	.	.	.	no
C32	C31	H31	109.52	.	.	.	no
C32	C31	H31'	109.47	.	.	.	no
H31'	C31	H31"	109.42	.	.	.	no
H32	C32	H32'	107.78	.	.	.	no
C233	C232	H232	121.9(12)	.	.	.	no
C31	C32	H32	109.03	.	.	.	no
C31	C32	H32'	109.07	.	.	.	no
C33	C32	H32	109.00	.	.	.	no

C33	C32	H32'	109.05	.	.	.	no
C231	C232	H232	116.8(12)	.	.	.	no
C32	C33	H33	108.58	.	.	.	no
C232	C233	H233	121.0(13)	.	.	.	no
C234	C233	H233	118.1(13)	.	.	.	no
C34	C33	H33	108.64	.	.	.	no
C34	C33	H33'	108.56	.	.	.	no
H33	C33	H33'	107.50	.	.	.	no
C32	C33	H33'	108.53	.	.	.	no
C33	C34	H34'	109.22	.	.	.	no
C35	C34	H34	109.12	.	.	.	no
C33	C34	H34	109.15	.	.	.	no
C233	C234	H234	121.7(13)	.	.	.	no
C235	C234	H234	119.5(13)	.	.	.	no
C35	C34	H34'	109.12	.	.	.	no
H34	C34	H34'	107.87	.	.	.	no
C234	C235	H235	118.7(11)	.	.	.	no
H35	C35	H35"	109.49	.	.	.	no
C236	C235	H235	120.7(10)	.	.	.	no
H35'	C35	H35"	109.49	.	.	.	no
C34	C35	H35	109.43	.	.	.	no
C34	C35	H35'	109.46	.	.	.	no
C34	C35	H35"	109.38	.	.	.	no
H35	C35	H35'	109.58	.	.	.	no
C235	C236	H236	120.9(11)	.	.	.	no
C231	C236	H236	117.5(11)	.	.	.	no
C41	C42	C43	123.2(7)	.	.	.	no
C42	C43	C44	113.6(6)	.	.	.	no
C43	C44	C45	116.4(8)	.	.	.	no
C42	C41	H41	109.47	.	.	.	no
C42	C41	H41'	109.43	.	.	.	no
C42	C41	H41"	109.40	.	.	.	no
H41	C41	H41'	109.54	.	.	.	no
H41	C41	H41"	109.53	.	.	.	no
H41'	C41	H41"	109.45	.	.	.	no
C41	C42	H42	106.57	.	.	.	no
C41	C42	H42'	106.54	.	.	.	no
C43	C42	H42	106.52	.	.	.	no
C43	C42	H42'	106.54	.	.	.	no
H42	C42	H42'	106.50	.	.	.	no
C42	C43	H43	108.81	.	.	.	no
C42	C43	H43'	108.82	.	.	.	no
C44	C43	H43	108.80	.	.	.	no
C44	C43	H43'	108.83	.	.	.	no
H43	C43	H43'	107.79	.	.	.	no
C43	C44	H44	108.17	.	.	.	no
C43	C44	H44'	108.21	.	.	.	no
C45	C44	H44	108.24	.	.	.	no
C45	C44	H44'	108.22	.	.	.	no
H44	C44	H44'	107.27	.	.	.	no
C44	C45	H45	109.51	.	.	.	no
C44	C45	H45'	109.41	.	.	.	no
C44	C45	H45"	109.48	.	.	.	no
H45	C45	H45'	109.45	.	.	.	no
H45	C45	H45"	109.58	.	.	.	no
H45'	C45	H45"	109.40	.	.	.	no

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N12	Fe11	N11	C16	165.09(10)	.	.	.	.	no
N12	Fe11	N11	C113	-12.54(11)	.	.	.	.	no
C130	Fe11	N11	C16	-14.63(13)	.	.	.	.	no
C130	Fe11	N11	C113	167.74(11)	.	.	.	.	no
N11	Fe11	N12	C116	11.55(12)	.	.	.	.	no
N11	Fe11	N12	C118	-166.91(10)	.	.	.	.	no
C130	Fe11	N12	C116	-168.74(11)	.	.	.	.	no
C130	Fe11	N12	C118	12.80(14)	.	.	.	.	no
N11	Fe11	C130	C131	54.83(16)	.	.	.	.	no
N12	Fe11	C130	C131	-124.79(12)	.	.	.	.	no
N21	Fe21	C230	C231	-51.38(16)	.	.	.	.	no
N22	Fe21	C230	C231	132.21(11)	.	.	.	.	no
N22	Fe21	N21	C213	9.94(12)	.	.	.	.	no
C230	Fe21	N22	C218	-16.32(13)	.	.	.	.	no
C230	Fe21	N22	C216	167.05(11)	.	.	.	.	no
N22	Fe21	N21	C26	-171.43(10)	.	.	.	.	no
C230	Fe21	N21	C213	-167.31(11)	.	.	.	.	no
N21	Fe21	N22	C216	-10.42(12)	.	.	.	.	no
C230	Fe21	N21	C26	11.32(14)	.	.	.	.	no
N21	Fe21	N22	C218	166.20(10)	.	.	.	.	no
Fe11	N11	C113	C114	-173.71(10)	.	.	.	.	no
C113	N11	C16	C11	97.12(15)	.	.	.	.	no
C113	N11	C16	C15	-87.75(17)	.	.	.	.	no
C16	N11	C113	C115	-171.33(13)	.	.	.	.	no
Fe11	N11	C113	C115	6.20(18)	.	.	.	.	no
C16	N11	C113	C114	8.76(19)	.	.	.	.	no
Fe11	N11	C16	C15	94.51(14)	.	.	.	.	no
Fe11	N11	C16	C11	-80.62(14)	.	.	.	.	no
C118	N12	C116	C115	174.11(14)	.	.	.	.	no
Fe11	N12	C116	C115	-4.3(2)	.	.	.	.	no
Fe11	N12	C116	C117	177.05(11)	.	.	.	.	no
C116	N12	C118	C119	92.24(17)	.	.	.	.	no
Fe11	N12	C118	C123	88.73(15)	.	.	.	.	no
Fe11	N12	C118	C119	-89.22(15)	.	.	.	.	no
C116	N12	C118	C123	-89.81(17)	.	.	.	.	no
C118	N12	C116	C117	-4.5(2)	.	.	.	.	no
C213	N21	C26	C21	-95.44(17)	.	.	.	.	no
Fe21	N21	C26	C21	85.87(14)	.	.	.	.	no
Fe21	N21	C26	C25	-88.88(14)	.	.	.	.	no
C26	N21	C213	C215	177.40(13)	.	.	.	.	no
Fe21	N21	C213	C215	-4.1(2)	.	.	.	.	no
C26	N21	C213	C214	-2.4(2)	.	.	.	.	no
Fe21	N21	C213	C214	176.13(11)	.	.	.	.	no
C213	N21	C26	C25	89.81(17)	.	.	.	.	no
Fe21	N22	C216	C215	5.1(2)	.	.	.	.	no
C216	N22	C218	C223	84.09(17)	.	.	.	.	no
C218	N22	C216	C217	8.5(2)	.	.	.	.	no
C218	N22	C216	C215	-171.42(13)	.	.	.	.	no
Fe21	N22	C216	C217	-175.04(12)	.	.	.	.	no
C216	N22	C218	C219	-100.33(16)	.	.	.	.	no
Fe21	N22	C218	C219	82.89(14)	.	.	.	.	no
Fe21	N22	C218	C223	-92.70(14)	.	.	.	.	no
C17	C11	C16	C15	-178.44(14)	.	.	.	.	no
C12	C11	C17	C18	93.4(2)	.	.	.	.	no
C17	C11	C16	N11	-3.4(2)	.	.	.	.	no
C16	C11	C17	C19	147.88(17)	.	.	.	.	no
C16	C11	C12	C13	-1.9(2)	.	.	.	.	no
C12	C11	C17	C19	-32.1(2)	.	.	.	.	no
C12	C11	C16	N11	176.61(13)	.	.	.	.	no
C16	C11	C17	C18	-86.6(2)	.	.	.	.	no

C17	C11	C12	C13	178.04(16)	.	.	.	.	no
C12	C11	C16	C15	1.5(2)	.	.	.	.	no
C11	C12	C13	C14	1.1(3)	.	.	.	.	no
C12	C13	C14	C15	0.2(3)	.	.	.	.	no
C13	C14	C15	C16	-0.5(2)	.	.	.	.	no
C13	C14	C15	C110	-178.22(16)	.	.	.	.	no
C14	C15	C110	C111	70.0(2)	.	.	.	.	no
C16	C15	C110	C111	-107.61(18)	.	.	.	.	no
C14	C15	C16	N11	-175.25(14)	.	.	.	.	no
C110	C15	C16	C11	177.27(14)	.	.	.	.	no
C14	C15	C16	C11	-0.3(2)	.	.	.	.	no
C14	C15	C110	C112	-53.5(2)	.	.	.	.	no
C16	C15	C110	C112	128.92(17)	.	.	.	.	no
C110	C15	C16	N11	2.4(2)	.	.	.	.	no
C112	C110	C111	H111	63.9(13)	.	.	.	.	no
H110	C110	C111	H111'	64.3(16)	.	.	.	.	no
H110	C110	C111	H111"	-58.9(15)	.	.	.	.	no
H110	C110	C111	H111	-179.2(16)	.	.	.	.	no
C15	C110	C112	H112'	-175.0(13)	.	.	.	.	no
C15	C110	C111	H111	-60.6(13)	.	.	.	.	no
C111	C110	C112	H112'	61.6(13)	.	.	.	.	no
C112	C110	C111	H111"	-175.7(12)	.	.	.	.	no
C111	C110	C112	H112	178.3(14)	.	.	.	.	no
H110	C110	C112	H112'	-55.6(16)	.	.	.	.	no
C111	C110	C112	H112"	-59.8(14)	.	.	.	.	no
C15	C110	C112	H112"	63.6(14)	.	.	.	.	no
C15	C110	C112	H112	-58.4(14)	.	.	.	.	no
C15	C110	C111	H111'	-177.1(13)	.	.	.	.	no
H110	C110	C112	H112	61.1(17)	.	.	.	.	no
C112	C110	C111	H111'	-52.5(13)	.	.	.	.	no
C15	C110	C111	H111"	59.7(12)	.	.	.	.	no
H110	C110	C112	H112"	-177.0(16)	.	.	.	.	no
C115	C113	C114	H114'	23.7(14)	.	.	.	.	no
C115	C113	C114	H114"	-94.7(15)	.	.	.	.	no
N11	C113	C115	H115	-179.2(12)	.	.	.	.	no
N11	C113	C114	H114"	85.2(15)	.	.	.	.	no
C115	C113	C114	H114	149.3(13)	.	.	.	.	no
N11	C113	C114	H114	-30.8(13)	.	.	.	.	no
N11	C113	C114	H114'	-156.4(14)	.	.	.	.	no
C114	C113	C115	H115	0.7(12)	.	.	.	.	no
H115	C115	C116	C117	-3.4(11)	.	.	.	.	no
H115	C115	C116	N12	178.0(11)	.	.	.	.	no
N12	C116	C117	H117"	62.9(17)	.	.	.	.	no
C115	C116	C117	H117	130.3(15)	.	.	.	.	no
N12	C116	C117	H117	-51.0(15)	.	.	.	.	no
N12	C116	C117	H117'	-172.1(16)	.	.	.	.	no
C115	C116	C117	H117"	-115.8(17)	.	.	.	.	no
C115	C116	C117	H117'	9.2(16)	.	.	.	.	no
C118	C119	C120	H120	178.1(12)	.	.	.	.	no
C124	C119	C120	H120	-2.9(12)	.	.	.	.	no
C120	C119	C124	H124	173.7(11)	.	.	.	.	no
C118	C119	C124	H124	-7.3(11)	.	.	.	.	no
H120	C120	C121	C122	-178.5(12)	.	.	.	.	no
H120	C120	C121	H121	-0.1(18)	.	.	.	.	no
C119	C120	C121	H121	177.8(13)	.	.	.	.	no
C27	C21	C22	C23	-179.73(16)	.	.	.	.	no
C22	C21	C26	N21	-173.26(14)	.	.	.	.	no
C22	C21	C26	C25	1.4(2)	.	.	.	.	no
C26	C21	C22	C23	-0.1(2)	.	.	.	.	no
C26	C21	C27	C28	-112.1(2)	.	.	.	.	no
C26	C21	C27	C29	125.3(2)	.	.	.	.	no
H121	C121	C122	H122	0(2)	.	.	.	.	no
C27	C21	C26	N21	6.3(2)	.	.	.	.	no
C27	C21	C26	C25	-179.01(14)	.	.	.	.	no



C22	C21	C27	C28	67.4(2)	.	.	.	.	no
C22	C21	C27	C29	-55.1(3)	.	.	.	.	no
C120	C121	C122	H122	178.0(14)	.	.	.	.	no
H121	C121	C122	C123	-177.8(14)	.	.	.	.	no
C21	C22	C23	C24	-1.0(3)	.	.	.	.	no
H122	C122	C123	C118	-177.6(13)	.	.	.	.	no
H122	C122	C123	C127	3.3(13)	.	.	.	.	no
C122	C123	C127	H127	-168.7(12)	.	.	.	.	no
C118	C123	C127	H127	12.3(12)	.	.	.	.	no
C22	C23	C24	C25	1.0(3)	.	.	.	.	no
C119	C124	C125	H125	-63.7(15)	.	.	.	.	no
C126	C124	C125	H125'	49.9(14)	.	.	.	.	no
C126	C124	C125	H125	171.0(15)	.	.	.	.	no
H124	C124	C125	H125'	-67.6(18)	.	.	.	.	no
C126	C124	C125	H125"	-67.2(16)	.	.	.	.	no
H124	C124	C125	H125	53.6(18)	.	.	.	.	no
C119	C124	C125	H125"	58.1(16)	.	.	.	.	no
H124	C124	C126	H126	169(2)	.	.	.	.	no
H124	C124	C126	H126"	-64(2)	.	.	.	.	no
C119	C124	C126	H126	-71.0(17)	.	.	.	.	no
C125	C124	C126	H126'	-62.2(17)	.	.	.	.	no
H124	C124	C125	H125"	175.4(19)	.	.	.	.	no
C23	C24	C25	C210	178.93(15)	.	.	.	.	no
C23	C24	C25	C26	0.3(2)	.	.	.	.	no
C119	C124	C126	H126'	173.2(16)	.	.	.	.	no
C119	C124	C126	H126"	56.2(17)	.	.	.	.	no
H124	C124	C126	H126'	53(2)	.	.	.	.	no
C125	C124	C126	H126"	-179.2(16)	.	.	.	.	no
C119	C124	C125	H125'	175.2(14)	.	.	.	.	no
C125	C124	C126	H126	53.5(17)	.	.	.	.	no
C210	C25	C26	C21	179.91(14)	.	.	.	.	no
C24	C25	C210	C211	-67.6(2)	.	.	.	.	no
C26	C25	C210	C211	111.00(18)	.	.	.	.	no
C24	C25	C210	C212	55.73(19)	.	.	.	.	no
C24	C25	C26	C21	-1.5(2)	.	.	.	.	no
C210	C25	C26	N21	-5.5(2)	.	.	.	.	no
C24	C25	C26	N21	173.16(13)	.	.	.	.	no
C26	C25	C210	C212	-125.67(16)	.	.	.	.	no
C123	C127	C128	H128	62.9(17)	.	.	.	.	no
C129	C127	C128	H128	-61.5(17)	.	.	.	.	no
C129	C127	C128	H128'	178.3(17)	.	.	.	.	no
C123	C127	C128	H128"	-175.9(13)	.	.	.	.	no
H127	C127	C128	H128	-179(2)	.	.	.	.	no
C129	C127	C128	H128"	59.8(13)	.	.	.	.	no
C123	C127	C129	H129"	-61.2(18)	.	.	.	.	no
C123	C127	C129	H129	178.0(15)	.	.	.	.	no
C123	C127	C129	H129'	55.9(15)	.	.	.	.	no
H127	C127	C128	H128'	61(2)	.	.	.	.	no
H127	C127	C128	H128"	-57.3(18)	.	.	.	.	no
C123	C127	C128	H128'	-57.3(17)	.	.	.	.	no
H127	C127	C129	H129"	-179(2)	.	.	.	.	no
H127	C127	C129	H129	59.8(19)	.	.	.	.	no
C128	C127	C129	H129"	64.0(18)	.	.	.	.	no
C128	C127	C129	H129	-56.8(15)	.	.	.	.	no
C128	C127	C129	H129'	-178.9(15)	.	.	.	.	no
H127	C127	C129	H129'	-62.3(19)	.	.	.	.	no
H130'	C130	C131	C132	-142.0(14)	.	.	.	.	no
H130'	C130	C131	C136	39.1(14)	.	.	.	.	no
H130	C130	C131	C132	-18.4(15)	.	.	.	.	no
H130	C130	C131	C136	162.7(15)	.	.	.	.	no
C130	C131	C136	H136	0.4(13)	.	.	.	.	no
C132	C131	C136	H136	-178.5(13)	.	.	.	.	no
C130	C131	C132	H132	2.3(15)	.	.	.	.	no
C136	C131	C132	H132	-178.8(14)	.	.	.	.	no

H132	C132	C133	H133	2(2)	.	.	.	.	no
H132	C132	C133	C134	178.1(15)	.	.	.	.	no
C131	C132	C133	H133	-176.7(16)	.	.	.	.	no
H133	C133	C134	C135	177.2(15)	.	.	.	.	no
H133	C133	C134	H134	2(2)	.	.	.	.	no
C132	C133	C134	H134	-174.3(16)	.	.	.	.	no
H134	C134	C135	H135	-5(2)	.	.	.	.	no
C133	C134	C135	H135	179.5(13)	.	.	.	.	no
H134	C134	C135	C136	174.7(16)	.	.	.	.	no
C134	C135	C136	H136	178.7(14)	.	.	.	.	no
H135	C135	C136	C131	179.9(13)	.	.	.	.	no
H135	C135	C136	H136	-1.1(19)	.	.	.	.	no
C214	C213	C215	C216	173.98(15)	.	.	.	.	no
N21	C213	C215	C216	-5.8(3)	.	.	.	.	no
C213	C215	C216	N22	5.3(3)	.	.	.	.	no
C213	C215	C216	C217	-174.61(16)	.	.	.	.	no
N22	C218	C223	C227	-1.8(2)	.	.	.	.	no
C219	C218	C223	C222	1.3(2)	.	.	.	.	no
C219	C218	C223	C227	-177.36(14)	.	.	.	.	no
N22	C218	C219	C224	5.2(2)	.	.	.	.	no
C223	C218	C219	C220	0.0(2)	.	.	.	.	no
N22	C218	C219	C220	-175.43(13)	.	.	.	.	no
N22	C218	C223	C222	176.84(14)	.	.	.	.	no
C223	C218	C219	C224	-179.35(14)	.	.	.	.	no
C224	C219	C220	C221	177.75(15)	.	.	.	.	no
C218	C219	C220	C221	-1.7(2)	.	.	.	.	no
C218	C219	C224	C226	-118.20(17)	.	.	.	.	no
C220	C219	C224	C225	-61.4(2)	.	.	.	.	no
C218	C219	C224	C225	117.99(17)	.	.	.	.	no
C220	C219	C224	C226	62.4(2)	.	.	.	.	no
C219	C220	C221	C222	1.9(3)	.	.	.	.	no
C220	C221	C222	C223	-0.4(3)	.	.	.	.	no
C221	C222	C223	C218	-1.1(2)	.	.	.	.	no
C221	C222	C223	C227	177.58(16)	.	.	.	.	no
C218	C223	C227	C228	-120.70(19)	.	.	.	.	no
C218	C223	C227	C229	115.3(2)	.	.	.	.	no
C222	C223	C227	C229	-63.3(2)	.	.	.	.	no
C222	C223	C227	C228	60.6(2)	.	.	.	.	no
Fe21	C230	C231	C236	74.61(17)	.	.	.	.	no
Fe21	C230	C231	C232	-104.05(16)	.	.	.	.	no
C230	C231	C232	C233	179.08(16)	.	.	.	.	no
C230	C231	C236	C235	-179.07(15)	.	.	.	.	no
C232	C231	C236	C235	-0.3(2)	.	.	.	.	no
C236	C231	C232	C233	0.4(2)	.	.	.	.	no
C31	C32	C33	C34	178.0(5)	.	.	.	.	no
C231	C232	C233	C234	0.1(3)	.	.	.	.	no
C232	C233	C234	C235	-0.5(3)	.	.	.	.	no
C32	C33	C34	C35	-178.6(5)	.	.	.	.	no
C233	C234	C235	C236	0.5(3)	.	.	.	.	no
C234	C235	C236	C231	-0.1(3)	.	.	.	.	no
C41	C42	C43	C44	178.6(8)	.	.	.	.	no
C42	C43	C44	C45	176.1(9)	.	.	.	.	no

loop_									
_geom_contact_atom_site_label_1									
_geom_contact_atom_site_label_2									
_geom_contact_distance									
_geom_contact_site_symmetry_1									
_geom_contact_site_symmetry_2									
_geom_contact_publ_flag									
Fe11	C17	3.6265(17)	.	.	.	.	.	.	no
Fe11	C110	4.0065(18)	.	.	.	.	.	.	no
Fe11	C124	3.8820(17)	.	.	.	.	.	.	no
Fe11	C127	3.8492(18)	.	.	.	.	.	.	no

Fe11	C129	3.998(3)	.	.	no
Fe21	C210	3.9006(16)	.	.	no
Fe21	C27	3.8300(17)	.	.	no
Fe21	C28	4.039(3)	.	.	no
Fe21	C224	3.7722(17)	.	.	no
Fe21	C227	3.9180(18)	.	.	no
Fe11	H111"	3.48(2)	.	.	no
Fe11	H136	3.516(18)	.	.	no
Fe11	H17	2.84(2)	.	.	no
Fe11	H124	3.349(17)	.	.	no
Fe11	H129'	3.31(2)	.	.	no
Fe11	H127	3.363(18)	.	.	no
Fe11	H125	3.35(2)	.	.	no
Fe21	H226"	3.48(2)	.	.	no
Fe21	H28"	3.39(3)	.	.	no
Fe21	H27	3.440(19)	.	.	no
Fe21	H224	3.228(17)	.	.	no
Fe21	H210	3.447(17)	.	.	no
Fe21	H211	3.45(2)	.	.	no
Fe21	H227	3.39(2)	.	.	no
Fe21	H236	3.473(18)	.	.	no
N11	H17	2.49(2)	.	.	no
N11	H110	2.493(17)	.	.	no
N11	H18'	2.93(3)	.	.	no
N12	H124	2.453(17)	.	.	no
N12	H127	2.442(18)	.	.	no
N21	H27	2.500(19)	.	.	no
N21	H210	2.491(16)	.	.	no
N22	H224	2.453(17)	.	.	no
N22	H227	2.433(19)	.	.	no
C11	C136	3.469(2)	.	.	no
C12	C136	3.577(2)	.	.	no
C12	C135	3.545(2)	.	.	no
C15	C114	3.336(2)	.	.	no
C17	C113	3.503(2)	.	.	no
C17	Fe11	3.6265(17)	.	.	no
C18	C113	3.537(4)	.	.	no
C21	C214	3.532(2)	.	.	no
C24	C220	3.512(2)	.	4_554	no
C25	C214	3.412(2)	.	.	no
C27	C213	3.536(2)	.	.	no
C27	Fe21	3.8300(17)	.	.	no
C28	Fe21	4.039(3)	.	.	no
C110	Fe11	4.0065(18)	.	.	no
C110	C113	3.476(2)	.	.	no
C110	C114	3.576(2)	.	.	no
C11	H114	3.03(2)	.	.	no
C12	H19	2.98(2)	.	.	no
C12	H19"	2.82(3)	.	.	no
C12	H18"	3.08(2)	.	.	no
C113	C110	3.476(2)	.	.	no
C113	C18	3.537(4)	.	.	no
C113	C17	3.503(2)	.	.	no
C14	H111	2.86(2)	.	.	no
C14	H112"	2.80(2)	.	.	no
C114	C110	3.576(2)	.	.	no
C114	C15	3.336(2)	.	.	no
C15	H114	2.98(2)	.	.	no
C16	H114	2.49(2)	.	.	no
C16	H18'	3.05(3)	.	.	no
C116	C127	3.463(2)	.	.	no
C116	C124	3.519(2)	.	.	no
C117	C123	3.406(2)	.	.	no
C117	C119	3.374(2)	.	.	no

C119	C117	3.374(2)	.	.	no
C19	H12	2.605(18)	.	.	no
C21	H214"	3.00(2)	.	.	no
C22	H234	3.04(2)	.	3_665	no
C22	H29"	2.71(3)	.	.	no
C22	H28	2.81(3)	.	.	no
C123	C117	3.406(2)	.	.	no
C23	H35"	3.0598	.	1_655	no
C23	H234	3.09(2)	.	3_665	no
C24	H211"	2.84(2)	.	.	no
C124	C116	3.519(2)	.	.	no
C124	Fe11	3.8820(17)	.	.	no
C24	H212	2.83(2)	.	.	no
C25	H236	3.079(18)	.	.	no
C25	H214	3.05(2)	.	.	no
C26	H214"	2.66(2)	.	.	no
C26	H214	2.85(2)	.	.	no
C127	Fe11	3.8492(18)	.	.	no
C127	C116	3.463(2)	.	.	no
C28	H22	3.013(18)	.	.	no
C29	H22	2.836(18)	.	.	no
C129	Fe11	3.998(3)	.	.	no
C31	H125'	2.97(2)	.	.	no
C135	C12	3.545(2)	.	.	no
C136	C11	3.469(2)	.	.	no
C136	C12	3.577(2)	.	.	no
C44	@28"	3.04(2)	.	2_645	no
C210	Fe21	3.9006(16)	.	.	no
C210	C213	3.477(2)	.	.	no
C111	H14	3.037(19)	.	.	no
C111	@28'	3.05(3)	.	4_554	no
C112	H14	2.79(2)	.	.	no
C113	H110	2.809(17)	.	.	no
C213	C210	3.477(2)	.	.	no
C113	H18'	2.69(3)	.	.	no
C213	C27	3.536(2)	.	.	no
C114	H110	3.091(16)	.	.	no
C114	H44	3.0048	.	3_655	no
C214	C21	3.532(2)	.	.	no
C114	H18'	2.74(3)	.	.	no
C214	C25	3.412(2)	.	.	no
C115	H29'	2.92(3)	.	2_645	no
C115	H232	2.974(19)	.	.	no
C116	H127	2.802(18)	.	.	no
C216	C227	3.382(2)	.	.	no
C116	H124	2.888(17)	.	.	no
C217	C223	3.405(2)	.	.	no
C217	C219	3.522(2)	.	.	no
C118	H117	2.65(2)	.	.	no
C118	H117"	2.73(2)	.	.	no
C219	C217	3.522(2)	.	.	no
C119	H117	2.85(2)	.	.	no
C120	H125"	2.91(2)	.	.	no
C120	H19"	3.05(3)	.	2_555	no
C120	H126	2.83(3)	.	.	no
C220	C24	3.512(2)	.	4_555	no
C121	@17'	2.94(3)	.	1_455	no
C122	H129"	2.92(3)	.	.	no
C122	@17'	2.92(3)	.	1_455	no
C122	H111	3.03(2)	.	4_555	no
C122	H128	2.76(3)	.	.	no
C223	C217	3.405(2)	.	.	no
C123	H117"	2.99(2)	.	.	no
C224	Fe21	3.7722(17)	.	.	no

C125	H233	3.05(2)	.	.	no
C125	H31	3.0877	.	.	no
C125	H120	3.059(18)	.	.	no
C126	H120	2.795(17)	.	.	no
C227	C216	3.382(2)	.	.	no
C227	Fe21	3.9180(18)	.	.	no
C128	H33'	3.0556	.	4_555	no
C128	H122	2.73(2)	.	.	no
C128	H29	3.01(4)	.	2_645	no
C129	H122	3.08(2)	.	.	no
C132	H210	3.078(16)	.	1_455	no
C133	H224	3.089(18)	.	1_455	no
C134	H13	2.98(2)	.	3_555	no
C134	H19	2.99(2)	.	.	no
C134	@11'	3.05(2)	.	1_455	no
C135	H19	3.07(2)	.	.	no
C136	@12'	2.85(2)	.	1_455	no
C211	H24	3.002(17)	.	.	no
C212	H122	2.99(2)	.	4_654	no
C212	H24	2.845(16)	.	.	no
C213	H210	2.822(17)	.	.	no
C213	H18	3.10(3)	.	2_655	no
C213	H27	2.898(19)	.	.	no
C214	H34'	2.9956	.	3_665	no
C215	H132	3.00(2)	.	1_655	no
C216	H227	2.740(19)	.	.	no
C216	H224	2.997(17)	.	.	no
C218	H217"	2.65(2)	.	.	no
C218	H217	2.72(3)	.	.	no
C219	H217"	2.97(2)	.	.	no
C220	H225	2.87(2)	.	.	no
C220	H226	2.83(2)	.	.	no
C220	H24	2.893(17)	.	4_555	no
C221	H117'	2.76(2)	.	.	no
C222	H117'	2.98(2)	.	.	no
C222	@11"	3.07(2)	.	4_555	no
C222	H229	2.81(3)	.	.	no
C222	H228"	2.79(2)	.	.	no
C223	H217	2.95(3)	.	.	no
C224	H133	3.01(2)	.	1_655	no
C225	H220	2.957(17)	.	.	no
C226	H133	3.09(2)	.	1_655	no
C226	H220	2.945(18)	.	.	no
C228	H222	2.884(18)	.	.	no
C228	H43	3.0366	.	2_655	no
C229	H222	2.960(19)	.	.	no
C230	H114"	3.10(2)	.	.	no
C230	H226"	2.99(2)	.	.	no
C231	H28"	2.96(3)	.	.	no
C232	H28"	2.98(3)	.	.	no
C232	H110	3.043(16)	.	.	no
C234	H111'	3.01(2)	.	.	no
C235	H22	3.034(18)	.	3_665	no
C236	H112'	2.86(2)	.	.	no
H111'	H112'	2.50(3)	.	.	no
H111'	C234	3.01(2)	.	.	no
H111"	Fe11	3.48(2)	.	.	no
H111"	H130'	2.59(3)	.	.	no
H112'	C236	2.86(2)	.	.	no
H112'	H111'	2.50(3)	.	.	no
H112"	H14	2.28(3)	.	.	no
H112"	H111	2.57(3)	.	.	no
H112"	C14	2.80(2)	.	.	no
H114'	H115	2.31(3)	.	.	no

H114"	C230	3.10(2)	.	.	no
H117'	H115	2.25(3)	.	.	no
H117'	C222	2.98(2)	.	.	no
H117'	C221	2.76(2)	.	.	no
H117"	C118	2.73(2)	.	.	no
H117"	C123	2.99(2)	.	.	no
H125'	H126'	2.46(3)	.	.	no
H125'	H233	2.52(3)	.	.	no
H125'	C31	2.97(2)	.	.	no
H125'	H31	2.5542	.	.	no
H125"	H19'	2.53(3)	.	2_555	no
H125"	C120	2.91(2)	.	.	no
H125"	H126	2.54(3)	.	.	no
H126'	H125'	2.46(3)	.	.	no
H12	H19"	2.16(3)	.	.	no
H12	C19	2.605(18)	.	.	no
H126"	H117	2.50(4)	.	.	no
H13	H134	2.35(3)	.	3_555	no
H13	C134	2.98(2)	.	3_555	no
H128'	C111	3.05(3)	.	4_555	no
H14	C112	2.79(2)	.	.	no
H14	H111	2.54(3)	.	.	no
H14	C111	3.037(19)	.	.	no
H14	H112"	2.28(3)	.	.	no
H128"	H29	2.57(5)	.	2_645	no
H128"	H33	2.4595	.	2_545	no
H128"	H129	2.52(3)	.	.	no
H129'	Fe11	3.31(2)	.	.	no
H129"	H128	2.52(4)	.	.	no
H129"	C122	2.92(3)	.	.	no
H17	N11	2.49(2)	.	.	no
H17	Fe11	2.84(2)	.	.	no
H130'	H111"	2.59(3)	.	.	no
H130'	H136	2.55(3)	.	.	no
H18	C213	3.10(3)	.	2_645	no
H18	H27	2.60(3)	.	2_645	no
H18	H19'	2.50(3)	.	.	no
H18'	C16	3.05(3)	.	.	no
H18'	H114	2.44(3)	.	.	no
H18'	N11	2.93(3)	.	.	no
H18'	C114	2.74(3)	.	.	no
H18'	C113	2.69(3)	.	.	no
H18"	C12	3.08(2)	.	.	no
H18"	H19"	2.36(4)	.	.	no
H211'	H212'	2.51(3)	.	.	no
H211'	C134	3.05(2)	.	1_655	no
H19	C134	2.99(2)	.	.	no
H19	C12	2.98(2)	.	.	no
H19	C135	3.07(2)	.	.	no
H19'	@25"	2.53(3)	.	2_545	no
H19'	H18	2.50(3)	.	.	no
H19"	C12	2.82(3)	.	.	no
H19"	H12	2.16(3)	.	.	no
H19"	H120	2.56(3)	.	2_545	no
H19"	H18"	2.36(4)	.	.	no
H19"	C120	3.05(3)	.	2_545	no
H211"	C222	3.07(2)	.	4_554	no
H211"	H212	2.54(3)	.	.	no
H211"	H24	2.47(3)	.	.	no
H211"	C24	2.84(2)	.	.	no
H212'	H211'	2.51(3)	.	.	no
H212'	H122	2.57(3)	.	4_654	no
H212'	C136	2.85(2)	.	1_655	no
H212"	H32	2.4995	.	3_665	no

H212"	H214	2.51(3)	.	.	no
H22	C29	2.836(18)	.	.	no
H22	H235	2.41(3)	.	3_665	no
H22	H29"	2.24(4)	.	.	no
H22	H28	2.44(4)	.	.	no
H22	C235	3.034(18)	.	3_665	no
H22	C28	3.013(18)	.	.	no
H214'	H215	2.29(3)	.	.	no
H23	H220	2.59(3)	.	4_554	no
H214"	C21	3.00(2)	.	.	no
H214"	C26	2.66(2)	.	.	no
H24	C211	3.002(17)	.	.	no
H24	C212	2.845(16)	.	.	no
H24	C220	2.893(17)	.	4_554	no
H24	H211"	2.47(3)	.	.	no
H24	H212	2.35(3)	.	.	no
H217'	C122	2.92(3)	.	1_655	no
H217'	H215	2.22(3)	.	.	no
H217'	C121	2.94(3)	.	1_655	no
H217"	C218	2.65(2)	.	.	no
H217"	H225'	2.50(3)	.	.	no
H217"	C219	2.97(2)	.	.	no
H225'	H217"	2.50(3)	.	.	no
H27	H18	2.60(3)	.	2_655	no
H27	C213	2.898(19)	.	.	no
H27	N21	2.500(19)	.	.	no
H27	Fe21	3.440(19)	.	.	no
H225"	H226'	2.51(3)	.	.	no
H28	H22	2.44(4)	.	.	no
H28	H29"	2.49(4)	.	.	no
H28	C22	2.81(3)	.	.	no
H28'	H29'	2.48(4)	.	.	no
H28"	C232	2.98(3)	.	.	no
H28"	C231	2.96(3)	.	.	no
H28"	Fe21	3.39(3)	.	.	no
H226'	H133	2.55(3)	.	1_655	no
H226'	H225"	2.51(3)	.	.	no
H29	C128	3.01(4)	.	2_655	no
H29	@28"	2.57(5)	.	2_655	no
H29'	H28'	2.48(4)	.	.	no
H29'	C115	2.92(3)	.	2_655	no
H29"	H22	2.24(4)	.	.	no
H29"	C22	2.71(3)	.	.	no
H29"	H28	2.49(4)	.	.	no
H226"	Fe21	3.48(2)	.	.	no
H226"	C230	2.99(2)	.	.	no
H226"	H230'	2.58(3)	.	.	no
H228'	H217	2.45(4)	.	.	no
H31	H125'	2.5542	.	.	no
H31	H33	2.5471	.	.	no
H31	C125	3.0877	.	.	no
H31"	H33'	2.5438	.	.	no
H228"	H222	2.33(3)	.	.	no
H228"	H44'	2.4056	.	2_655	no
H228"	H43'	2.4281	.	4_555	no
H228"	C222	2.79(2)	.	.	no
H228"	C44	3.04(2)	.	2_655	no
H32	@12"	2.4995	.	3_665	no
H32	H34	2.5465	.	.	no
H32'	H34'	2.5996	.	.	no
H33	H35"	2.4630	.	.	no
H33	@28"	2.4595	.	2_555	no
H33	H31	2.5471	.	.	no
H33'	C128	3.0556	.	4_554	no

H33'	H128	2.4908	.	4_554	no
H33'	H31"	2.5438	.	.	no
H33'	H35	2.5402	.	.	no
H34	H32	2.5465	.	.	no
H34'	H32'	2.5996	.	.	no
H34'	C214	2.9956	.	3_665	no
H230'	H232	2.38(3)	.	.	no
H230'	H226"	2.58(3)	.	.	no
H35	H33'	2.5402	.	.	no
H35"	H33	2.4630	.	.	no
H35"	C23	3.0598	.	1_455	no
H42	H44'	2.4720	.	.	no
H42'	H44	2.5119	.	.	no
H43	C228	3.0366	.	2_645	no
H43	H228	2.5850	.	2_645	no
H43	H45	2.4134	.	.	no
H43'	H45"	2.5080	.	.	no
H43'	@28"	2.4281	.	4_554	no
H44	C114	3.0048	.	3_655	no
H44	H42'	2.5119	.	.	no
H44'	H42	2.4720	.	.	no
H44'	H112	2.4900	.	3_655	no
H44'	@28"	2.4056	.	2_645	no
H45	H43	2.4134	.	.	no
H45"	H43'	2.5080	.	.	no
H110	C114	3.091(16)	.	.	no
H110	C113	2.809(17)	.	.	no
H110	C232	3.043(16)	.	.	no
H110	N11	2.493(17)	.	.	no
H111	H112"	2.57(3)	.	.	no
H111	H14	2.54(3)	.	.	no
H111	C122	3.03(2)	.	4_554	no
H111	C14	2.86(2)	.	.	no
H112	H44'	2.4900	.	3_655	no
H114	H18'	2.44(3)	.	.	no
H114	C15	2.98(2)	.	.	no
H114	C16	2.49(2)	.	.	no
H114	C11	3.03(2)	.	.	no
H115	H114'	2.31(3)	.	.	no
H115	H117'	2.25(3)	.	.	no
H117	H126"	2.50(4)	.	.	no
H117	C119	2.85(2)	.	.	no
H117	C118	2.65(2)	.	.	no
H120	C126	2.795(17)	.	.	no
H120	H126	2.31(3)	.	.	no
H120	H19"	2.56(3)	.	2_555	no
H120	C125	3.059(18)	.	.	no
H122	C129	3.08(2)	.	.	no
H122	H128	2.18(3)	.	.	no
H122	C128	2.73(2)	.	.	no
H122	@12'	2.57(3)	.	4_455	no
H122	C212	2.99(2)	.	4_455	no
H124	Fe11	3.349(17)	.	.	no
H124	C116	2.888(17)	.	.	no
H124	N12	2.453(17)	.	.	no
H125	Fe11	3.35(2)	.	.	no
H126	C120	2.83(3)	.	.	no
H126	H125"	2.54(3)	.	.	no
H126	H120	2.31(3)	.	.	no
H127	Fe11	3.363(18)	.	.	no
H127	N12	2.442(18)	.	.	no
H127	C116	2.802(18)	.	.	no
H128	H122	2.18(3)	.	.	no
H128	H129"	2.52(4)	.	.	no



H128	H33'	2.4908	.	4_555	no
H128	C122	2.76(3)	.	.	no
H129	H128"	2.52(3)	.	.	no
H130	H132	2.39(3)	.	.	no
H132	C215	3.00(2)	.	1_455	no
H132	H130	2.39(3)	.	.	no
H133	H224	2.40(3)	.	1_455	no
H133	C226	3.09(2)	.	1_455	no
H133	C224	3.01(2)	.	1_455	no
H133	@26'	2.55(3)	.	1_455	no
H134	H13	2.35(3)	.	3_555	no
H136	H130'	2.55(3)	.	.	no
H136	Fe11	3.516(18)	.	.	no
H210	Fe21	3.447(17)	.	.	no
H210	N21	2.491(16)	.	.	no
H210	C213	2.822(17)	.	.	no
H210	C132	3.078(16)	.	1_655	no
H211	Fe21	3.45(2)	.	.	no
H212	C24	2.83(2)	.	.	no
H212	H211"	2.54(3)	.	.	no
H212	H24	2.35(3)	.	.	no
H214	H212"	2.51(3)	.	.	no
H214	C25	3.05(2)	.	.	no
H214	C26	2.85(2)	.	.	no
H215	H217'	2.22(3)	.	.	no
H215	H214'	2.29(3)	.	.	no
H217	C218	2.72(3)	.	.	no
H217	C223	2.95(3)	.	.	no
H217	H228'	2.45(4)	.	.	no
H220	H23	2.59(3)	.	4_555	no
H220	H225	2.46(3)	.	.	no
H220	H226	2.44(3)	.	.	no
H220	C225	2.957(17)	.	.	no
H220	C226	2.945(18)	.	.	no
H222	H229	2.45(3)	.	.	no
H222	H228"	2.33(3)	.	.	no
H222	C228	2.884(18)	.	.	no
H222	C229	2.960(19)	.	.	no
H224	C133	3.089(18)	.	1_655	no
H224	C216	2.997(17)	.	.	no
H224	H133	2.40(3)	.	1_655	no
H224	N22	2.453(17)	.	.	no
H224	Fe21	3.228(17)	.	.	no
H225	C220	2.87(2)	.	.	no
H225	H226	2.54(3)	.	.	no
H225	H220	2.46(3)	.	.	no
H226	C220	2.83(2)	.	.	no
H226	H225	2.54(3)	.	.	no
H226	H220	2.44(3)	.	.	no
H227	N22	2.433(19)	.	.	no
H227	Fe21	3.39(2)	.	.	no
H227	C216	2.740(19)	.	.	no
H228	H43	2.5850	.	2_655	no
H229	C222	2.81(3)	.	.	no
H229	H222	2.45(3)	.	.	no
H230	H236	2.57(3)	.	.	no
H232	H230'	2.38(3)	.	.	no
H232	C115	2.974(19)	.	.	no
H233	C125	3.05(2)	.	.	no
H233	H125'	2.52(3)	.	.	no
H234	C22	3.04(2)	.	3_665	no
H234	C23	3.09(2)	.	3_665	no
H235	H22	2.41(3)	.	3_665	no
H236	C25	3.079(18)	.	.	no

H236	H230	2.57(3)	.	.	no
H236	Fe21	3.473(18)	.	.	no

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#D   H   A   D - H   H...A   D...A   D - H...A   symm(A)
#
C17   H17   N11       1.00(2)   2.49(2)   2.862(2)   101.8(13)   .   yes
C27   H27   N21       0.917(18)  2.500(19)  2.929(2)   108.9(13)   .   yes
C110  H110  N11       0.973(17)  2.493(17)  2.951(2)   108.6(11)   .   yes
C124  H124  N12       0.956(17)  2.453(17)  2.928(2)   110.5(12)   .   yes
C127  H127  N12       0.952(18)  2.442(18)  2.911(2)   110.2(13)   .   yes
C210  H210  N21       0.955(18)  2.491(16)  2.942(2)   108.9(11)   .   yes
C224  H224  N22       0.961(17)  2.453(17)  2.933(2)   110.7(12)   .   yes
C227  H227  N22       0.927(19)  2.433(19)  2.917(2)   112.6(14)   .   yes

```

===END of Crystallographic Information File

data\_c54h48bf

\_database\_code\_CSD 185603

```

_audit_creation_date      '2001-11-08 16:04:43'
_audit_creation_method    'PLATON <TABLE ACC> option'
_audit_update_record
;
?
;

```

=====

## # 5. CHEMICAL DATA

```

_chemical_name_systematic
;
?
;
_chemical_name_common      ?
_chemical_melting_point    ?
_chemical_formula_moiety    'C54 H48 B F15 Fe N2'
_chemical_formula_structural ?
_chemical_formula_sum       'C54 H48 B F15 Fe N2'
_chemical_formula_weight    1076.62
_chemical_compound_source   'see text'

```

```

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
N   N   0.0061   0.0033
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

```

```

Fe Fe    0.3463    0.8444
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
F  F     0.0171    0.0103
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
B  B     0.0013    0.0007
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H  H     0.0000    0.0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C  C     0.0033    0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

```

```

#=====

```

# ``` # 6. CRYSTAL DATA ```

```

_symmetry_cell_setting      Monoclinic
_symmetry_space_group_name_Hall '-C 2yc'
_symmetry_space_group_name_H-M 'C 2/c'

```

```

loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x,y,1/2-z
-x,-y,-z
x,-y,1/2+z
1/2+x,1/2+y,z
1/2-x,1/2+y,1/2-z
1/2-x,1/2-y,-z
1/2+x,1/2-y,1/2+z

```

```

_cell_length_a              44.806(3)
_cell_length_b              13.349(1)
_cell_length_c              17.780(1)
_cell_angle_alpha           90
_cell_angle_beta            113.282(5)
_cell_angle_gamma           90
_cell_volume                9768.5(12)
_cell_formula_units_Z       8

```

```

_cell_measurement_temperature 110(1)
_cell_measurement_reflns_used 1379
_cell_measurement_theta_min 2.29
_cell_measurement_theta_max 17.85
_cell_special_details
;

```

The final unit cell was obtained from the xyz centroids of 1379 reflections after integration using the SAINT software package (Bruker, 2000).

```

;

```

```

_exptl_crystal_description 'platelet'
_exptl_crystal_colour      'red-orange'
_exptl_crystal_size_max    0.15
_exptl_crystal_size_mid    0.14
_exptl_crystal_size_min    0.08
_exptl_crystal_size_rad    ?
_exptl_crystal_density_meas ?
_exptl_crystal_density_diffn 1.464
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000       4416
_exptl_absorpt_coefficient_mu 0.406
_exptl_absorpt_correction_type 'Multi-Scan'
_exptl_absorpt_process_details '(SADABS, Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min 0.9416

```

\_exptl\_absorpt\_correction\_T\_max 0.9682

#=====

## # 7. EXPERIMENTAL DATA

\_exptl\_special\_details

;  
?  
;

\_diffrn\_ambient\_temperature 110(2)  
\_diffrn\_radiation\_wavelength 0.71073  
\_diffrn\_radiation\_type MoK $\alpha$   
\_diffrn\_radiation\_source 'fine focus sealed Siemens Mo tube '  
\_diffrn\_radiation\_monochromator 'parallel mounted graphite'  
\_diffrn\_radiation\_detector

;

CCD area-detector

;

\_diffrn\_measurement\_device\_type

;

Bruker Smart Apex

;

\_diffrn\_measurement\_method 'phi and omega scans'

\_diffrn\_special\_details

;

Crystal into the cold nitrogen stream of the low-temperature  
unit (KRYOFLEX, (Bruker, 2000)).

;

\_diffrn\_detector\_area\_resol\_mean '4096x4096 / 62x62 (binned 512)'

\_diffrn\_standards\_number ?

\_diffrn\_standards\_interval\_count ?

\_diffrn\_standards\_interval\_time ?

loop\_

\_diffrn\_standard\_refl\_index\_h

\_diffrn\_standard\_refl\_index\_k

\_diffrn\_standard\_refl\_index\_l

? ? ?

# number of measured reflections (redundant set)

\_diffrn\_reflns\_number 34522

\_diffrn\_reflns\_av\_R\_equivalents 0.3431

\_diffrn\_reflns\_av\_sigmaI/netI 0.4426

\_diffrn\_reflns\_limit\_h\_min -58

\_diffrn\_reflns\_limit\_h\_max 58

\_diffrn\_reflns\_limit\_k\_min -17

\_diffrn\_reflns\_limit\_k\_max 17

\_diffrn\_reflns\_limit\_l\_min -23

\_diffrn\_reflns\_limit\_l\_max 22

\_diffrn\_reflns\_theta\_min 2.29

\_diffrn\_reflns\_theta\_max 27.50

\_diffrn\_measured\_fraction\_theta\_max 0.997

\_diffrn\_reflns\_theta\_full 27.50

\_diffrn\_measured\_fraction\_theta\_full 0.997

\_diffrn\_reflns\_reduction\_process

;

Intensity data were corrected for Lorentz and polarization  
effects, decay and absorption and reduced to  $F_o \sim 2^2$   
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)

```

;

# number of unique reflections
_reflns_number_total      11209
_reflns_number_gt        3022
_reflns_threshold_expression >2sigma(I)

_computing_data_collection      'SMART, Bruker Version 5.264, 2001'
_computing_cell_refinement      'SAINT, Bruker Version 6.02A, 2000'
_computing_data_reduction      'XPREP, Bruker Version 5.1/NT, 2000'
_computing_structure_solution
;
SIR-97 (Altomare et al., 1997)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2001)
PLATON (Spek, 1994)
;
_computing_publication_material
;
PLATON (Spek, 1990)
SHELXL (Sheldrick, 1997)
;

#=====

# 8. REFINEMENT DATA

_refine_special_details
;
Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type           full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
'calc w=1/[s2(Fo2)+(0.0338P)2+0.0000P] where P=(Fo2+2Fc2)/3'
_atom_sites_solution_primary     direct
_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
_refine_ls_hydrogen_treatment    refall
_refine_ls_extinction_method     SHELXL
_refine_ls_extinction_coef       0.00050(7)
_refine_ls_extinction_expression ?
_refine_ls_abs_structure_details ?
_refine_ls_abs_structure_Flack   ?
_refine_ls_number_reflns         11209
_refine_ls_number_parameters     851
_refine_ls_number_restraints     0
_refine_ls_number_constraints    ?
_refine_ls_R_factor_all          0.3106
_refine_ls_R_factor_gt           0.0678
_refine_ls_wR_factor_ref         0.1767

```

\_refine\_ls\_wR\_factor\_gt 0.1095  
\_refine\_ls\_goodness\_of\_fit\_ref 0.869  
\_refine\_ls\_restrained\_S\_all 0.869  
\_refine\_ls\_shift/su\_max 0.158  
\_refine\_ls\_shift/su\_mean 0.000

\_refine\_diff\_density\_max 0.427  
\_refine\_diff\_density\_min -0.511  
\_refine\_diff\_density\_rms 0.082  
\_vrn\_publ\_code\_void\_volume 71.0  
\_vrn\_publ\_code\_meas\_time 13.5

#=====

# # 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

loop\_  
\_atom\_site\_label  
\_atom\_site\_type\_symbol  
\_atom\_site\_thermal\_displace\_type  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z  
\_atom\_site\_occupancy  
\_atom\_site\_U\_iso\_or\_equiv  
\_atom\_site\_calc\_flag  
\_atom\_site\_refinement\_flags  
Fe Fe Uani 0.12880(2) 0.28531(8) 0.15337(6) 1.000 0.0281(4) . .  
F1 F Uani 0.16941(9) -0.0124(3) 0.3673(2) 1.000 0.0395(17) . .  
F2 F Uani 0.23329(10) -0.0231(3) 0.4177(3) 1.000 0.0571(19) . .  
F3 F Uani 0.27324(9) 0.1030(3) 0.5345(3) 1.000 0.0495(16) . .  
F4 F Uani 0.24638(9) 0.2421(3) 0.6016(2) 1.000 0.0484(17) . .  
F5 F Uani 0.18280(9) 0.2538(3) 0.5541(2) 1.000 0.0389(16) . .  
F6 F Uani 0.16099(9) 0.0785(3) 0.6040(2) 1.000 0.0379(16) . .  
F7 F Uani 0.13773(11) 0.1209(3) 0.7156(2) 1.000 0.0523(19) . .  
F8 F Uani 0.08345(11) 0.2359(3) 0.6776(3) 1.000 0.070(2) . .  
F9 F Uani 0.05288(10) 0.3079(3) 0.5213(3) 1.000 0.0603(19) . .  
F10 F Uani 0.07445(9) 0.2649(3) 0.4080(2) 1.000 0.0511(18) . .  
F11 F Uani 0.15115(9) -0.0734(3) 0.4928(2) 1.000 0.0396(17) . .  
F12 F Uani 0.11839(10) -0.2416(3) 0.4414(3) 1.000 0.0515(17) . .  
F13 F Uani 0.05996(10) -0.2419(3) 0.3105(2) 1.000 0.0522(17) . .  
F14 F Uani 0.03490(10) -0.0635(3) 0.2358(3) 1.000 0.0576(19) . .  
F15 F Uani 0.06596(9) 0.1048(3) 0.2874(2) 1.000 0.0484(17) . .  
N1 N Uani 0.08413(12) 0.3306(4) 0.0882(3) 1.000 0.029(2) . .  
N2 N Uani 0.15047(12) 0.3921(4) 0.1169(3) 1.000 0.025(2) . .  
C1 C Uani 0.05740(15) 0.2940(6) 0.1094(4) 1.000 0.028(3) . .  
C2 C Uani 0.04978(16) 0.3511(6) 0.1664(4) 1.000 0.032(3) . .  
C3 C Uani 0.02537(18) 0.3141(7) 0.1878(5) 1.000 0.041(3) . .  
C4 C Uani 0.0090(2) 0.2261(7) 0.1570(5) 1.000 0.043(3) . .  
C5 C Uani 0.0172(2) 0.1743(7) 0.1020(5) 1.000 0.043(3) . .  
C6 C Uani 0.04181(15) 0.2051(6) 0.0774(4) 1.000 0.031(3) . .  
C7 C Uani 0.0652(2) 0.4519(6) 0.2000(5) 1.000 0.041(3) . .  
C8 C Uani 0.0742(3) 0.4654(9) 0.2916(6) 1.000 0.050(4) . .  
C9 C Uani 0.0405(3) 0.5368(9) 0.1577(7) 1.000 0.077(5) . .  
C10 C Uani 0.04873(19) 0.1427(7) 0.0135(5) 1.000 0.042(3) . .  
C11 C Uani 0.0547(3) 0.0308(8) 0.0363(8) 1.000 0.057(4) . .  
C12 C Uani 0.0205(3) 0.1511(11) -0.0686(6) 1.000 0.063(5) . .  
C13 C Uani 0.07723(16) 0.3974(5) 0.0269(4) 1.000 0.029(3) . .  
C14 C Uani 0.04207(18) 0.4184(7) -0.0290(5) 1.000 0.035(3) . .  
C15 C Uani 0.10056(17) 0.4522(6) 0.0117(5) 1.000 0.034(3) . .  
C16 C Uani 0.13429(17) 0.4559(5) 0.0554(4) 1.000 0.028(3) . .  
C17 C Uani 0.1514(2) 0.5402(7) 0.0343(6) 1.000 0.040(3) . .  
C18 C Uani 0.18492(16) 0.4121(5) 0.1649(4) 1.000 0.028(3) . .  
C19 C Uani 0.20848(17) 0.3556(5) 0.1496(4) 1.000 0.029(3) . .

C20 C Uani 0.24083(18) 0.3732(6) 0.2007(5) 1.000 0.034(3) . .  
C21 C Uani 0.25010(19) 0.4373(6) 0.2662(5) 1.000 0.038(3) . .  
C22 C Uani 0.2265(2) 0.4903(7) 0.2799(5) 1.000 0.043(3) . .  
C23 C Uani 0.19322(17) 0.4813(5) 0.2294(4) 1.000 0.030(3) . .  
C24 C Uani 0.19898(17) 0.2832(6) 0.0783(4) 1.000 0.035(3) . .  
C25 C Uani 0.2235(2) 0.1953(7) 0.0947(6) 1.000 0.044(4) . .  
C26 C Uani 0.1939(2) 0.3343(7) -0.0026(5) 1.000 0.043(3) . .  
C27 C Uani 0.1680(2) 0.5444(7) 0.2465(5) 1.000 0.043(3) . .  
C28 C Uani 0.1776(3) 0.6543(7) 0.2596(6) 1.000 0.050(4) . .  
C29 C Uani 0.1602(2) 0.5032(8) 0.3162(6) 1.000 0.044(4) . .  
C30 C Uani 0.1217(2) 0.1433(6) 0.2221(4) 1.000 0.033(3) . .  
C31 C Uani 0.1358(2) 0.1118(6) 0.1696(5) 1.000 0.036(3) . .  
C32 C Uani 0.16793(18) 0.1335(5) 0.1846(4) 1.000 0.029(3) . .  
C33 C Uani 0.18553(17) 0.1934(5) 0.2519(4) 1.000 0.032(3) . .  
C34 C Uani 0.17103(19) 0.2266(6) 0.3042(5) 1.000 0.031(3) . .  
C35 C Uani 0.13956(15) 0.1999(5) 0.2934(4) 1.000 0.023(2) . .  
C36 C Uani 0.12517(18) 0.2224(6) 0.3535(4) 1.000 0.026(3) . .  
C37 C Uani 0.17168(16) 0.1173(5) 0.4611(4) 1.000 0.026(3) . .  
C38 C Uani 0.18756(17) 0.0515(5) 0.4289(4) 1.000 0.032(3) . .  
C39 C Uani 0.22065(18) 0.0459(6) 0.4524(5) 1.000 0.037(3) . .  
C40 C Uani 0.24089(18) 0.1068(6) 0.5114(5) 1.000 0.039(3) . .  
C41 C Uani 0.22720(18) 0.1752(6) 0.5450(4) 1.000 0.035(3) . .  
C42 C Uani 0.19374(18) 0.1801(5) 0.5185(4) 1.000 0.032(3) . .  
C43 C Uani 0.11971(17) 0.1689(5) 0.4980(4) 1.000 0.031(3) . .  
C44 C Uani 0.13384(17) 0.1363(5) 0.5796(4) 1.000 0.030(3) . .  
C45 C Uani 0.12236(19) 0.1579(6) 0.6386(4) 1.000 0.036(3) . .  
C46 C Uani 0.0949(2) 0.2147(6) 0.6191(5) 1.000 0.048(3) . .  
C47 C Uani 0.07976(17) 0.2510(5) 0.5414(5) 1.000 0.038(3) . .  
C48 C Uani 0.09172(18) 0.2268(6) 0.4836(4) 1.000 0.040(3) . .  
C49 C Uani 0.11191(16) 0.0267(6) 0.3913(4) 1.000 0.030(3) . .  
C50 C Uani 0.12222(17) -0.0664(6) 0.4274(4) 1.000 0.032(3) . .  
C51 C Uani 0.10582(19) -0.1541(6) 0.4015(5) 1.000 0.037(3) . .  
C52 C Uani 0.0768(2) -0.1545(7) 0.3365(5) 1.000 0.042(3) . .  
C53 C Uani 0.06408(18) -0.0673(7) 0.2992(5) 1.000 0.041(3) . .  
C54 C Uani 0.08119(18) 0.0204(6) 0.3275(4) 1.000 0.035(3) . .  
B B Uani 0.13225(18) 0.1334(6) 0.4263(5) 1.000 0.029(3) . .  
H3 H Uiso 0.0210(12) 0.353(4) 0.221(3) 1.000 0.030(16) . .  
H4 H Uiso -0.0066(14) 0.199(5) 0.174(4) 1.000 0.03(2) . .  
H5 H Uiso 0.0077(15) 0.125(5) 0.085(4) 1.000 0.03(2) . .  
H7 H Uiso 0.0773(17) 0.485(5) 0.168(4) 1.000 0.06(3) . .  
H8 H Uiso 0.0542(16) 0.453(5) 0.299(4) 1.000 0.04(2) . .  
H8' H Uiso 0.089(2) 0.527(6) 0.305(5) 1.000 0.09(3) . .  
H8" H Uiso 0.0891(17) 0.421(5) 0.307(4) 1.000 0.05(3) . .  
H9 H Uiso 0.0372(16) 0.534(5) 0.096(5) 1.000 0.06(3) . .  
H9' H Uiso 0.055(2) 0.624(7) 0.178(5) 1.000 0.12(4) . .  
H9" H Uiso 0.026(2) 0.530(8) 0.181(6) 1.000 0.11(5) . .  
H10 H Uiso 0.0678(13) 0.173(4) 0.016(3) 1.000 0.020(18) . .  
H11 H Uiso 0.067(3) 0.032(11) 0.079(8) 1.000 0.21(8) . .  
H11' H Uiso 0.0621(19) -0.020(6) -0.006(5) 1.000 0.09(3) . .  
H11" H Uiso 0.0319(14) 0.001(4) 0.036(3) 1.000 0.026(18) . .  
H12 H Uiso 0.0004(16) 0.135(5) -0.076(4) 1.000 0.04(2) . .  
H12' H Uiso 0.0271(12) 0.107(4) -0.102(3) 1.000 0.017(17) . .  
H12" H Uiso 0.0193(18) 0.220(6) -0.093(5) 1.000 0.07(3) . .  
H14 H Uiso 0.0249(15) 0.368(5) -0.007(4) 1.000 0.05(2) . .  
H14' H Uiso 0.0379(18) 0.405(6) -0.082(5) 1.000 0.08(3) . .  
H14" H Uiso 0.0400(12) 0.490(4) -0.026(3) 1.000 0.018(18) . .  
H15 H Uiso 0.0943(12) 0.502(4) -0.042(3) 1.000 0.022(17) . .  
H17 H Uiso 0.1500(14) 0.600(5) 0.060(4) 1.000 0.03(2) . .  
H17' H Uiso 0.1413(18) 0.549(6) -0.023(5) 1.000 0.08(3) . .  
H17" H Uiso 0.1744(18) 0.534(5) 0.045(4) 1.000 0.06(3) . .  
H20 H Uiso 0.2574(11) 0.337(3) 0.185(3) 1.000 0.030(14) . .  
H21 H Uiso 0.2727(16) 0.448(5) 0.304(4) 1.000 0.05(2) . .  
H22 H Uiso 0.234(2) 0.551(7) 0.320(6) 1.000 0.13(4) . .  
H24 H Uiso 0.1784(12) 0.257(4) 0.073(3) 1.000 0.016(16) . .

H25 H Uiso 0.2421(12) 0.212(4) 0.083(3) 1.000 0.017(16) . .  
 H25' H Uiso 0.2119(16) 0.158(5) 0.050(4) 1.000 0.05(3) . .  
 H25" H Uiso 0.2310(12) 0.161(4) 0.156(3) 1.000 0.016(16) . .  
 H26 H Uiso 0.169(3) 0.365(10) -0.012(8) 1.000 0.24(7) . .  
 H26' H Uiso 0.1866(11) 0.282(4) -0.047(3) 1.000 0.016(16) . .  
 H26" H Uiso 0.2130(14) 0.368(4) 0.000(3) 1.000 0.026(19) . .  
 H27 H Uiso 0.1524(13) 0.542(4) 0.202(3) 1.000 0.019(19) . .  
 H28 H Uiso 0.2008(12) 0.674(4) 0.311(3) 1.000 0.016(16) . .  
 H28' H Uiso 0.1595(19) 0.690(6) 0.266(5) 1.000 0.08(3) . .  
 H28" H Uiso 0.1837(13) 0.690(4) 0.219(3) 1.000 0.019(18) . .  
 H29 H Uiso 0.1518(18) 0.437(6) 0.304(5) 1.000 0.07(3) . .  
 H29' H Uiso 0.143(2) 0.549(6) 0.342(5) 1.000 0.12(3) . .  
 H29" H Uiso 0.1821(15) 0.502(4) 0.365(4) 1.000 0.04(2) . .  
 H30 H Uiso 0.1029(14) 0.126(5) 0.215(4) 1.000 0.03(2) . .  
 H31 H Uiso 0.1288(14) 0.076(4) 0.134(4) 1.000 0.02(2) . .  
 H32 H Uiso 0.1792(12) 0.104(4) 0.147(3) 1.000 0.017(16) . .  
 H33 H Uiso 0.2112(12) 0.200(4) 0.263(3) 1.000 0.015(15) . .  
 H34 H Uiso 0.1780(14) 0.261(4) 0.343(3) 1.000 0.02(2) . .  
 H36 H Uiso 0.1003(14) 0.237(4) 0.324(3) 1.000 0.04(2) . .  
 H36' H Uiso 0.1330(13) 0.279(4) 0.383(3) 1.000 0.019(19) . .

loop\_

\_atom\_site\_aniso\_label  
 \_atom\_site\_aniso\_U\_11  
 \_atom\_site\_aniso\_U\_22  
 \_atom\_site\_aniso\_U\_33  
 \_atom\_site\_aniso\_U\_23  
 \_atom\_site\_aniso\_U\_13  
 \_atom\_site\_aniso\_U\_12

Fe 0.0284(6) 0.0338(7) 0.0214(6) 0.0039(6) 0.0090(5) 0.0003(5)  
 F1 0.043(3) 0.046(3) 0.030(3) -0.011(2) 0.015(2) 0.005(2)  
 F2 0.046(3) 0.077(4) 0.054(3) -0.003(3) 0.026(2) 0.019(3)  
 F3 0.023(2) 0.064(3) 0.053(3) 0.015(2) 0.006(2) 0.005(2)  
 F4 0.042(3) 0.045(3) 0.048(3) 0.001(2) 0.007(2) -0.011(2)  
 F5 0.040(2) 0.032(3) 0.044(3) -0.007(2) 0.016(2) 0.000(2)  
 F6 0.052(3) 0.043(3) 0.022(2) 0.009(2) 0.018(2) 0.006(2)  
 F7 0.092(4) 0.047(3) 0.022(3) 0.005(2) 0.027(3) 0.011(3)  
 F8 0.103(4) 0.080(4) 0.050(3) 0.013(3) 0.055(3) 0.026(3)  
 F9 0.057(3) 0.084(4) 0.047(3) 0.002(3) 0.028(2) 0.021(3)  
 F10 0.041(2) 0.081(4) 0.035(3) 0.011(3) 0.019(2) 0.019(2)  
 F11 0.042(3) 0.039(3) 0.026(3) 0.009(2) 0.001(2) -0.001(2)  
 F12 0.064(3) 0.032(3) 0.052(3) 0.001(2) 0.016(2) -0.002(2)  
 F13 0.068(3) 0.046(3) 0.045(3) -0.012(2) 0.025(2) -0.027(2)  
 F14 0.038(3) 0.078(4) 0.038(3) 0.000(3) -0.005(2) -0.013(3)  
 F15 0.035(3) 0.054(3) 0.045(3) 0.014(2) 0.004(2) -0.001(2)  
 N1 0.029(3) 0.034(4) 0.025(4) 0.007(3) 0.011(3) 0.003(3)  
 N2 0.025(3) 0.027(4) 0.021(4) 0.003(3) 0.008(3) 0.000(3)  
 C1 0.024(4) 0.036(5) 0.019(4) -0.002(4) 0.002(3) 0.000(4)  
 C2 0.032(4) 0.040(5) 0.021(5) 0.003(4) 0.008(4) -0.003(4)  
 C3 0.037(5) 0.060(7) 0.041(6) -0.003(5) 0.030(5) 0.000(5)  
 C4 0.041(5) 0.057(7) 0.032(5) -0.006(5) 0.016(4) -0.009(5)  
 C5 0.043(5) 0.051(7) 0.041(6) -0.009(5) 0.023(5) -0.019(5)  
 C6 0.022(4) 0.056(6) 0.015(4) -0.008(4) 0.006(3) -0.008(4)  
 C7 0.061(6) 0.040(6) 0.028(5) -0.004(4) 0.024(5) -0.009(5)  
 C8 0.043(7) 0.063(8) 0.033(6) 0.005(5) 0.003(5) 0.009(6)  
 C9 0.111(11) 0.065(9) 0.039(8) 0.015(6) 0.013(7) 0.012(8)  
 C10 0.038(5) 0.050(6) 0.042(6) -0.023(5) 0.021(5) -0.025(5)  
 C11 0.047(6) 0.053(8) 0.075(8) -0.025(6) 0.027(6) -0.009(5)  
 C12 0.058(8) 0.104(11) 0.029(6) -0.026(7) 0.019(6) -0.025(7)  
 C13 0.031(4) 0.032(5) 0.021(5) -0.001(4) 0.007(4) 0.003(4)  
 C14 0.029(5) 0.044(6) 0.023(5) 0.008(5) 0.001(4) -0.005(4)  
 C15 0.030(4) 0.033(5) 0.031(5) 0.007(4) 0.004(4) -0.003(4)  
 C16 0.034(4) 0.033(5) 0.017(4) 0.004(4) 0.009(4) 0.000(4)  
 C17 0.045(6) 0.040(6) 0.028(6) 0.011(5) 0.006(5) 0.000(5)



```

C18 0.024(4) 0.032(5) 0.022(4) 0.012(4) 0.003(3) -0.002(4)
C19 0.033(4) 0.033(5) 0.025(5) 0.006(4) 0.017(4) 0.003(4)
C20 0.026(4) 0.040(5) 0.037(5) 0.013(4) 0.015(4) 0.000(4)
C21 0.024(4) 0.056(6) 0.026(5) 0.007(5) 0.001(4) -0.012(4)
C22 0.039(5) 0.041(6) 0.034(6) 0.002(5) 0.000(4) -0.010(4)
C23 0.035(5) 0.028(5) 0.027(5) 0.006(4) 0.012(4) 0.006(4)
C24 0.029(4) 0.050(6) 0.032(5) 0.000(5) 0.019(4) -0.004(4)
C25 0.024(5) 0.059(7) 0.053(7) -0.004(6) 0.021(5) 0.004(5)
C26 0.049(6) 0.054(7) 0.026(5) 0.001(5) 0.016(5) -0.020(5)
C27 0.044(5) 0.047(6) 0.024(6) 0.002(5) 0.000(5) 0.004(5)
C28 0.075(7) 0.029(6) 0.041(6) -0.005(5) 0.018(6) -0.009(6)
C29 0.052(6) 0.046(7) 0.037(6) -0.008(5) 0.021(5) 0.000(5)
C30 0.031(5) 0.047(6) 0.021(5) -0.002(4) 0.011(4) 0.003(4)
C31 0.043(6) 0.029(5) 0.038(6) -0.002(5) 0.018(5) -0.004(4)
C32 0.045(5) 0.035(5) 0.017(4) 0.004(4) 0.022(4) -0.001(4)
C33 0.037(5) 0.034(5) 0.022(4) 0.009(4) 0.010(4) -0.002(4)
C34 0.046(5) 0.031(5) 0.020(5) 0.000(4) 0.018(4) -0.007(4)
C35 0.027(4) 0.026(4) 0.012(4) 0.003(4) 0.002(3) -0.001(4)
C36 0.036(5) 0.025(5) 0.015(4) 0.007(4) 0.009(4) 0.002(4)
C37 0.034(4) 0.029(5) 0.017(4) 0.006(4) 0.011(4) -0.005(4)
C38 0.041(5) 0.035(5) 0.018(4) -0.002(4) 0.011(4) -0.009(4)
C39 0.031(5) 0.045(6) 0.039(5) 0.002(5) 0.018(4) 0.009(4)
C40 0.030(5) 0.053(6) 0.034(5) 0.022(5) 0.013(4) 0.004(4)
C41 0.035(5) 0.034(5) 0.027(5) 0.003(4) 0.002(4) 0.002(4)
C42 0.046(5) 0.031(5) 0.023(5) 0.005(4) 0.017(4) 0.000(4)
C43 0.037(4) 0.030(5) 0.026(5) -0.006(4) 0.013(4) -0.006(4)
C44 0.027(4) 0.033(5) 0.026(5) -0.003(4) 0.006(4) 0.000(4)
C45 0.051(5) 0.039(5) 0.021(5) 0.000(4) 0.016(4) 0.006(4)
C46 0.077(6) 0.045(5) 0.038(5) 0.000(5) 0.041(5) 0.008(5)
C47 0.036(5) 0.039(5) 0.046(5) 0.008(4) 0.025(4) 0.013(4)
C48 0.044(5) 0.058(6) 0.016(4) 0.006(4) 0.009(4) -0.004(5)
C49 0.025(4) 0.043(5) 0.022(5) 0.001(4) 0.010(4) -0.004(4)
C50 0.032(4) 0.035(5) 0.022(5) -0.007(4) 0.003(4) -0.004(4)
C51 0.047(5) 0.035(5) 0.027(5) 0.007(4) 0.014(4) 0.004(4)
C52 0.051(6) 0.049(6) 0.031(5) -0.011(5) 0.022(5) -0.023(5)
C53 0.032(5) 0.060(7) 0.032(5) -0.002(5) 0.013(4) -0.014(5)
C54 0.034(5) 0.038(5) 0.031(5) 0.014(4) 0.012(4) 0.014(4)
B 0.023(5) 0.028(6) 0.028(5) 0.004(4) 0.002(4) 0.005(4)

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#=====

# # 10. MOLECULAR GEOMETRY

\_geom\_special\_details

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Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All esds are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

;

loop\_

\_geom\_bond\_atom\_site\_label\_1

\_geom\_bond\_atom\_site\_label\_2

\_geom\_bond\_distance

\_geom\_bond\_site\_symmetry\_1

\_geom\_bond\_site\_symmetry\_2

\_geom\_bond\_publ\_flag

Fe	N1	1.970(6)	.	.	yes
Fe	N2	1.973(6)	.	.	yes
Fe	C30	2.344(8)	.	.	yes
Fe	C31	2.340(8)	.	.	yes
F1	C38	1.373(8)	.	.	yes

F2	C39	1.351(9)	.	.	yes
F3	C40	1.342(10)	.	.	yes
F4	C41	1.366(8)	.	.	yes
F5	C42	1.362(8)	.	.	yes
F6	C44	1.359(9)	.	.	yes
F7	C45	1.359(8)	.	.	yes
F8	C46	1.359(10)	.	.	yes
F9	C47	1.347(9)	.	.	yes
F10	C48	1.357(8)	.	.	yes
F11	C50	1.360(8)	.	.	yes
F12	C51	1.367(9)	.	.	yes
F13	C52	1.367(10)	.	.	yes
F14	C53	1.348(10)	.	.	yes
F15	C54	1.363(9)	.	.	yes
N1	C1	1.474(9)	.	.	yes
N1	C13	1.346(8)	.	.	yes
N2	C16	1.349(8)	.	.	yes
N2	C18	1.463(9)	.	.	yes
C1	C2	1.414(10)	.	.	no
C1	C6	1.381(11)	.	.	no
C2	C3	1.383(12)	.	.	no
C2	C7	1.523(11)	.	.	no
C3	C4	1.379(13)	.	.	no
C4	C5	1.361(13)	.	.	no
C5	C6	1.399(12)	.	.	no
C6	C10	1.536(11)	.	.	no
C7	C8	1.526(13)	.	.	no
C7	C9	1.555(15)	.	.	no
C10	C11	1.543(14)	.	.	no
C10	C12	1.511(14)	.	.	no
C13	C14	1.520(11)	.	.	no
C13	C15	1.387(11)	.	.	no
C15	C16	1.401(11)	.	.	no
C16	C17	1.491(12)	.	.	no
C18	C19	1.409(11)	.	.	no
C18	C23	1.403(9)	.	.	no
C19	C20	1.393(11)	.	.	no
C19	C24	1.515(10)	.	.	no
C20	C21	1.371(11)	.	.	no
C21	C22	1.372(13)	.	.	no
C22	C23	1.409(12)	.	.	no
C23	C27	1.533(12)	.	.	no
C24	C25	1.554(12)	.	.	no
C24	C26	1.526(11)	.	.	no
C27	C28	1.521(13)	.	.	no
C27	C29	1.517(13)	.	.	no
C30	C31	1.383(12)	.	.	no
C30	C35	1.420(10)	.	.	no
C31	C32	1.387(13)	.	.	no
C32	C33	1.395(9)	.	.	no
C33	C34	1.400(11)	.	.	no
C34	C35	1.392(12)	.	.	no
C35	C36	1.481(10)	.	.	no
C36	B	1.692(11)	.	.	yes
C37	C38	1.388(10)	.	.	no
C37	C42	1.387(10)	.	.	no
C37	B	1.639(12)	.	.	yes
C38	C39	1.374(12)	.	.	no
C39	C40	1.353(12)	.	.	no
C40	C41	1.363(12)	.	.	no
C41	C42	1.384(12)	.	.	no
C43	C44	1.403(9)	.	.	no
C43	C48	1.408(11)	.	.	no
C43	B	1.653(11)	.	.	yes

C44	C45	1.369(11)	.	.	no
C45	C46	1.368(12)	.	.	no
C46	C47	1.365(11)	.	.	no
C47	C48	1.372(11)	.	.	no
C49	C50	1.391(11)	.	.	no
C49	C54	1.398(10)	.	.	no
C49	B	1.673(11)	.	.	yes
C50	C51	1.362(11)	.	.	no
C51	C52	1.356(12)	.	.	no
C52	C53	1.349(13)	.	.	no
C53	C54	1.381(12)	.	.	no
C3	H3	0.86(5)	.	.	no
C4	H4	0.94(7)	.	.	no
C5	H5	0.78(7)	.	.	no
C7	H7	1.03(8)	.	.	no
C8	H8	0.97(8)	.	.	no
C8	H8'	1.02(9)	.	.	no
C8	H8"	0.85(8)	.	.	no
C9	H9	1.05(8)	.	.	no
C9	H9'	1.31(10)	.	.	no
C9	H9"	0.90(10)	.	.	no
C10	H10	0.93(6)	.	.	no
C11	H11	0.74(14)	.	.	no
C11	H11'	1.15(8)	.	.	no
C11	H11"	1.09(7)	.	.	no
C12	H12	0.88(8)	.	.	no
C12	H12'	0.96(5)	.	.	no
C12	H12"	1.01(8)	.	.	no
C14	H14	1.20(7)	.	.	no
C14	H14'	0.90(8)	.	.	no
C14	H14"	0.96(5)	.	.	no
C15	H15	1.10(5)	.	.	no
C17	H17	0.93(7)	.	.	no
C17	H17'	0.94(8)	.	.	no
C17	H17"	0.97(9)	.	.	no
C20	H20	1.01(5)	.	.	no
C21	H21	0.98(7)	.	.	no
C22	H22	1.04(10)	.	.	no
C24	H24	0.96(6)	.	.	no
C25	H25	0.96(6)	.	.	no
C25	H25'	0.91(6)	.	.	no
C25	H25"	1.10(5)	.	.	no
C26	H26	1.14(14)	.	.	no
C26	H26'	1.01(5)	.	.	no
C26	H26"	0.95(7)	.	.	no
C27	H27	0.82(5)	.	.	no
C28	H28	1.11(6)	.	.	no
C28	H28'	0.99(9)	.	.	no
C28	H28"	0.99(6)	.	.	no
C29	H29	0.95(8)	.	.	no
C29	H29'	1.21(9)	.	.	no
C29	H29"	1.02(7)	.	.	no
C30	H30	0.83(7)	.	.	no
C31	H31	0.76(6)	.	.	no
C32	H32	1.06(5)	.	.	no
C33	H33	1.09(6)	.	.	no
C34	H34	0.78(5)	.	.	no
C36	H36	1.05(6)	.	.	no
C36	H36'	0.91(5)	.	.	no

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loop_
  _geom_angle_atom_site_label_1
  _geom_angle_atom_site_label_2
  _geom_angle_atom_site_label_3

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				_geom_angle				
				_geom_angle_site_symmetry_1				
				_geom_angle_site_symmetry_2				
				_geom_angle_site_symmetry_3				
				_geom_angle_publ_flag				
N1	Fe	N2	95.9(2)	.	.	.	yes	
N1	Fe	C30	103.8(3)	.	.	.	yes	
N1	Fe	C31	115.6(3)	.	.	.	yes	
N2	Fe	C30	160.3(3)	.	.	.	yes	
N2	Fe	C31	134.1(3)	.	.	.	yes	
C30	Fe	C31	34.4(3)	.	.	.	yes	
Fe	N1	C1	119.2(4)	.	.	.	yes	
Fe	N1	C13	122.3(5)	.	.	.	yes	
C1	N1	C13	118.5(6)	.	.	.	yes	
Fe	N2	C16	123.1(5)	.	.	.	yes	
Fe	N2	C18	118.9(4)	.	.	.	yes	
C16	N2	C18	117.6(6)	.	.	.	yes	
N1	C1	C2	117.1(6)	.	.	.	yes	
N1	C1	C6	120.6(6)	.	.	.	yes	
C2	C1	C6	122.2(7)	.	.	.	no	
C1	C2	C3	116.5(7)	.	.	.	no	
C1	C2	C7	123.9(7)	.	.	.	no	
C3	C2	C7	119.5(7)	.	.	.	no	
C2	C3	C4	123.3(8)	.	.	.	no	
C3	C4	C5	117.8(9)	.	.	.	no	
C4	C5	C6	123.0(8)	.	.	.	no	
C1	C6	C5	117.2(7)	.	.	.	no	
C1	C6	C10	123.6(7)	.	.	.	no	
C5	C6	C10	119.1(7)	.	.	.	no	
C2	C7	C8	114.2(7)	.	.	.	no	
C2	C7	C9	109.2(8)	.	.	.	no	
C8	C7	C9	105.5(8)	.	.	.	no	
C6	C10	C11	113.3(8)	.	.	.	no	
C6	C10	C12	109.7(8)	.	.	.	no	
C11	C10	C12	108.5(9)	.	.	.	no	
N1	C13	C14	119.9(7)	.	.	.	yes	
N1	C13	C15	123.9(7)	.	.	.	yes	
C14	C13	C15	116.2(7)	.	.	.	no	
C13	C15	C16	129.9(7)	.	.	.	no	
N2	C16	C15	122.9(7)	.	.	.	yes	
N2	C16	C17	121.0(7)	.	.	.	yes	
C15	C16	C17	115.9(7)	.	.	.	no	
N2	C18	C19	119.2(6)	.	.	.	yes	
N2	C18	C23	118.3(6)	.	.	.	yes	
C19	C18	C23	122.2(7)	.	.	.	no	
C18	C19	C20	116.7(6)	.	.	.	no	
C18	C19	C24	121.3(7)	.	.	.	no	
C20	C19	C24	121.9(7)	.	.	.	no	
C19	C20	C21	123.2(8)	.	.	.	no	
C20	C21	C22	118.5(8)	.	.	.	no	
C21	C22	C23	122.6(8)	.	.	.	no	
C18	C23	C22	116.7(7)	.	.	.	no	
C18	C23	C27	123.1(7)	.	.	.	no	
C22	C23	C27	120.3(7)	.	.	.	no	
C19	C24	C25	112.4(6)	.	.	.	no	
C19	C24	C26	113.1(7)	.	.	.	no	
C25	C24	C26	110.2(7)	.	.	.	no	
C23	C27	C28	112.0(8)	.	.	.	no	
C23	C27	C29	112.9(7)	.	.	.	no	
C28	C27	C29	111.5(8)	.	.	.	no	
Fe	C30	C31	72.6(5)	.	.	.	yes	
Fe	C30	C35	83.7(5)	.	.	.	yes	
C31	C30	C35	121.2(8)	.	.	.	no	
Fe	C31	C30	73.0(5)	.	.	.	yes	

Fe	C31	C32	84.0(5)	.	.	.	yes
C30	C31	C32	121.5(7)	.	.	.	no
C31	C32	C33	118.4(7)	.	.	.	no
C32	C33	C34	119.8(8)	.	.	.	no
C33	C34	C35	122.5(7)	.	.	.	no
C30	C35	C34	116.2(7)	.	.	.	no
C30	C35	C36	120.0(7)	.	.	.	no
C34	C35	C36	123.7(6)	.	.	.	no
C35	C36	B	114.0(6)	.	.	.	yes
C38	C37	C42	110.7(7)	.	.	.	no
C38	C37	B	125.4(6)	.	.	.	yes
C42	C37	B	123.2(6)	.	.	.	yes
F1	C38	C37	118.9(7)	.	.	.	yes
F1	C38	C39	115.9(6)	.	.	.	yes
C37	C38	C39	125.2(7)	.	.	.	no
F2	C39	C38	119.7(7)	.	.	.	yes
F2	C39	C40	119.3(8)	.	.	.	yes
C38	C39	C40	121.0(8)	.	.	.	no
F3	C40	C39	121.7(7)	.	.	.	yes
F3	C40	C41	120.7(7)	.	.	.	yes
C39	C40	C41	117.5(8)	.	.	.	no
F4	C41	C40	120.0(7)	.	.	.	yes
F4	C41	C42	120.1(7)	.	.	.	yes
C40	C41	C42	119.8(7)	.	.	.	no
F5	C42	C37	119.7(7)	.	.	.	yes
F5	C42	C41	114.6(6)	.	.	.	yes
C37	C42	C41	125.7(7)	.	.	.	no
C44	C43	C48	111.3(6)	.	.	.	no
C44	C43	B	123.8(7)	.	.	.	yes
C48	C43	B	124.6(6)	.	.	.	yes
F6	C44	C43	119.2(6)	.	.	.	yes
F6	C44	C45	115.8(6)	.	.	.	yes
C43	C44	C45	125.0(7)	.	.	.	no
F7	C45	C44	120.1(7)	.	.	.	yes
F7	C45	C46	120.2(7)	.	.	.	yes
C44	C45	C46	119.7(7)	.	.	.	no
F8	C46	C45	119.7(7)	.	.	.	yes
F8	C46	C47	120.9(8)	.	.	.	yes
C45	C46	C47	119.4(8)	.	.	.	no
F9	C47	C46	120.2(7)	.	.	.	yes
F9	C47	C48	120.5(7)	.	.	.	yes
C46	C47	C48	119.3(8)	.	.	.	no
F10	C48	C43	120.3(6)	.	.	.	yes
F10	C48	C47	114.5(7)	.	.	.	yes
C43	C48	C47	125.2(7)	.	.	.	no
C50	C49	C54	111.2(7)	.	.	.	no
C50	C49	B	123.8(6)	.	.	.	yes
C54	C49	B	124.8(7)	.	.	.	yes
F11	C50	C49	119.1(7)	.	.	.	yes
F11	C50	C51	115.8(7)	.	.	.	yes
C49	C50	C51	125.1(7)	.	.	.	no
F12	C51	C50	120.2(7)	.	.	.	yes
F12	C51	C52	119.9(7)	.	.	.	yes
C50	C51	C52	119.9(8)	.	.	.	no
F13	C52	C51	120.5(8)	.	.	.	yes
F13	C52	C53	120.0(8)	.	.	.	yes
C51	C52	C53	119.5(8)	.	.	.	no
F14	C53	C52	121.7(8)	.	.	.	yes
F14	C53	C54	119.2(8)	.	.	.	yes
C52	C53	C54	119.1(8)	.	.	.	no
F15	C54	C49	120.2(7)	.	.	.	yes
F15	C54	C53	114.8(7)	.	.	.	yes
C49	C54	C53	125.0(7)	.	.	.	no
C4	C3	H3	124(4)	.	.	.	no

C2	C3	H3	113(4)	.	.	.	no
C3	C4	H4	123(4)	.	.	.	no
C5	C4	H4	119(4)	.	.	.	no
C6	C5	H5	120(5)	.	.	.	no
C4	C5	H5	117(5)	.	.	.	no
C2	C7	H7	115(4)	.	.	.	no
C9	C7	H7	81(4)	.	.	.	no
C8	C7	H7	124(4)	.	.	.	no
C7	C8	H8'	103(5)	.	.	.	no
C7	C8	H8"	96(4)	.	.	.	no
H8	C8	H8"	119(6)	.	.	.	no
H8'	C8	H8"	98(7)	.	.	.	no
H8	C8	H8'	131(6)	.	.	.	no
C7	C8	H8	105(4)	.	.	.	no
C7	C9	H9'	109(4)	.	.	.	no
C7	C9	H9"	102(7)	.	.	.	no
H9	C9	H9'	100(5)	.	.	.	no
H9	C9	H9"	130(8)	.	.	.	no
H9'	C9	H9"	109(8)	.	.	.	no
C7	C9	H9	105(4)	.	.	.	no
C6	C10	H10	100(3)	.	.	.	no
C12	C10	H10	115(3)	.	.	.	no
C11	C10	H10	110(3)	.	.	.	no
C10	C11	H11"	107(3)	.	.	.	no
H11	C11	H11'	113(11)	.	.	.	no
H11'	C11	H11"	107(5)	.	.	.	no
C10	C11	H11	103(11)	.	.	.	no
H11	C11	H11"	109(11)	.	.	.	no
C10	C11	H11'	118(4)	.	.	.	no
C10	C12	H12	123(4)	.	.	.	no
C10	C12	H12"	111(5)	.	.	.	no
H12	C12	H12'	108(6)	.	.	.	no
H12	C12	H12"	106(7)	.	.	.	no
H12'	C12	H12"	106(6)	.	.	.	no
C10	C12	H12'	102(3)	.	.	.	no
C13	C14	H14	108(3)	.	.	.	no
C13	C14	H14'	112(5)	.	.	.	no
H14	C14	H14"	117(5)	.	.	.	no
H14'	C14	H14"	106(6)	.	.	.	no
C13	C14	H14"	104(3)	.	.	.	no
H14	C14	H14'	110(6)	.	.	.	no
C13	C15	H15	122(3)	.	.	.	no
C16	C15	H15	108(3)	.	.	.	no
C16	C17	H17'	107(5)	.	.	.	no
C16	C17	H17	112(4)	.	.	.	no
H17	C17	H17'	109(6)	.	.	.	no
H17	C17	H17"	104(6)	.	.	.	no
H17'	C17	H17"	104(7)	.	.	.	no
C16	C17	H17"	120(4)	.	.	.	no
C21	C20	H20	122(3)	.	.	.	no
C19	C20	H20	115(3)	.	.	.	no
C20	C21	H21	124(4)	.	.	.	no
C22	C21	H21	118(4)	.	.	.	no
C21	C22	H22	117(5)	.	.	.	no
C23	C22	H22	118(5)	.	.	.	no
C19	C24	H24	105(3)	.	.	.	no
C26	C24	H24	107(3)	.	.	.	no
C25	C24	H24	109(3)	.	.	.	no
C24	C25	H25'	98(5)	.	.	.	no
C24	C25	H25"	115(3)	.	.	.	no
H25	C25	H25'	101(6)	.	.	.	no
C24	C25	H25	113(3)	.	.	.	no
H25'	C25	H25"	119(5)	.	.	.	no
H25	C25	H25"	111(4)	.	.	.	no

C24	C26	H26	94(7)	.	.	.	no
C24	C26	H26'	108(3)	.	.	.	no
H26	C26	H26'	98(7)	.	.	.	no
H26	C26	H26"	130(8)	.	.	.	no
C24	C26	H26"	112(3)	.	.	.	no
H26'	C26	H26"	112(4)	.	.	.	no
C29	C27	H27	113(4)	.	.	.	no
C28	C27	H27	105(4)	.	.	.	no
C23	C27	H27	102(4)	.	.	.	no
C27	C28	H28	118(3)	.	.	.	no
H28	C28	H28'	110(6)	.	.	.	no
C27	C28	H28'	107(5)	.	.	.	no
C27	C28	H28"	120(3)	.	.	.	no
H28'	C28	H28"	109(6)	.	.	.	no
H28	C28	H28"	93(4)	.	.	.	no
C27	C29	H29	110(5)	.	.	.	no
C27	C29	H29'	121(4)	.	.	.	no
H29	C29	H29'	108(7)	.	.	.	no
H29	C29	H29"	110(6)	.	.	.	no
C27	C29	H29"	104(4)	.	.	.	no
H29'	C29	H29"	103(5)	.	.	.	no
C31	C30	H30	121(5)	.	.	.	no
C35	C30	H30	118(5)	.	.	.	no
Fe	C30	H30	119(5)	.	.	.	no
C30	C31	H31	127(5)	.	.	.	no
Fe	C31	H31	122(5)	.	.	.	no
C32	C31	H31	110(5)	.	.	.	no
C31	C32	H32	121(3)	.	.	.	no
C33	C32	H32	120(3)	.	.	.	no
C34	C33	H33	126(3)	.	.	.	no
C32	C33	H33	114(3)	.	.	.	no
C33	C34	H34	130(5)	.	.	.	no
C35	C34	H34	108(5)	.	.	.	no
C35	C36	H36'	114(4)	.	.	.	no
B	C36	H36	111(3)	.	.	.	no
C35	C36	H36	111(3)	.	.	.	no
H36	C36	H36'	103(5)	.	.	.	no
B	C36	H36'	103(3)	.	.	.	no
C36	B	C43	111.8(6)	.	.	.	yes
C36	B	C49	113.8(6)	.	.	.	yes
C37	B	C49	112.1(6)	.	.	.	yes
C43	B	C49	103.3(6)	.	.	.	yes
C37	B	C43	113.0(6)	.	.	.	yes
C36	B	C37	103.2(6)	.	.	.	yes

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N2	Fe	N1	C1	-162.6(5)	.	.	no
N2	Fe	N1	C13	14.5(5)	.	.	no
C30	Fe	N1	C1	17.3(5)	.	.	no
C30	Fe	N1	C13	-165.6(5)	.	.	no
C31	Fe	N1	C1	51.8(5)	.	.	no
C31	Fe	N1	C13	-131.1(5)	.	.	no
N1	Fe	N2	C16	-9.5(5)	.	.	no
N1	Fe	N2	C18	162.3(5)	.	.	no

C31	Fe	N2	C16	125.3(6)	.	.	.	.	no
C31	Fe	N2	C18	-62.9(6)	.	.	.	.	no
N1	Fe	C30	C31	115.3(5)	.	.	.	.	no
N1	Fe	C30	C35	-119.2(5)	.	.	.	.	no
C31	Fe	C30	C35	125.5(8)	.	.	.	.	no
N1	Fe	C31	C30	-76.7(5)	.	.	.	.	no
N1	Fe	C31	C32	157.7(4)	.	.	.	.	no
N2	Fe	C31	C30	154.8(4)	.	.	.	.	no
N2	Fe	C31	C32	29.2(6)	.	.	.	.	no
C30	Fe	C31	C32	-125.6(7)	.	.	.	.	no
C31	Fe	C30	H30	-117(5)	.	.	.	.	no
N1	Fe	C31	H31	47(6)	.	.	.	.	no
N2	Fe	C31	H31	-81(6)	.	.	.	.	no
C30	Fe	C31	H31	124(6)	.	.	.	.	no
N1	Fe	C30	H30	-1(5)	.	.	.	.	no
Fe	N1	C13	C15	-10.5(9)	.	.	.	.	no
C1	N1	C13	C14	-11.6(9)	.	.	.	.	no
Fe	N1	C13	C14	171.3(5)	.	.	.	.	no
Fe	N1	C1	C2	89.9(7)	.	.	.	.	no
Fe	N1	C1	C6	-87.0(7)	.	.	.	.	no
C13	N1	C1	C2	-87.3(8)	.	.	.	.	no
C13	N1	C1	C6	95.8(8)	.	.	.	.	no
C1	N1	C13	C15	166.6(7)	.	.	.	.	no
Fe	N2	C18	C19	85.8(7)	.	.	.	.	no
Fe	N2	C18	C23	-88.8(7)	.	.	.	.	no
Fe	N2	C16	C15	0.0(9)	.	.	.	.	no
Fe	N2	C16	C17	175.3(6)	.	.	.	.	no
C18	N2	C16	C15	-171.9(7)	.	.	.	.	no
C18	N2	C16	C17	3.4(10)	.	.	.	.	no
C16	N2	C18	C19	-101.9(7)	.	.	.	.	no
C16	N2	C18	C23	83.5(8)	.	.	.	.	no
C6	C1	C2	C7	-176.9(7)	.	.	.	.	no
C2	C1	C6	C5	1.7(11)	.	.	.	.	no
N1	C1	C6	C5	178.5(6)	.	.	.	.	no
N1	C1	C6	C10	-5.1(11)	.	.	.	.	no
N1	C1	C2	C3	-177.9(6)	.	.	.	.	no
N1	C1	C2	C7	6.2(10)	.	.	.	.	no
C6	C1	C2	C3	-1.0(11)	.	.	.	.	no
C2	C1	C6	C10	178.1(7)	.	.	.	.	no
C3	C2	C7	C8	46.1(11)	.	.	.	.	no
C3	C2	C7	C9	-71.7(10)	.	.	.	.	no
C1	C2	C3	C4	0.5(12)	.	.	.	.	no
C7	C2	C3	C4	176.6(8)	.	.	.	.	no
C1	C2	C7	C8	-138.1(9)	.	.	.	.	no
C1	C2	C7	C9	104.1(9)	.	.	.	.	no
C2	C3	C4	C5	-0.9(13)	.	.	.	.	no
C3	C4	C5	C6	1.6(13)	.	.	.	.	no
C4	C5	C6	C1	-2.1(12)	.	.	.	.	no
C4	C5	C6	C10	-178.6(8)	.	.	.	.	no
C5	C6	C10	C11	-53.0(11)	.	.	.	.	no
C5	C6	C10	C12	68.4(11)	.	.	.	.	no
C1	C6	C10	C12	-107.9(10)	.	.	.	.	no
C1	C6	C10	C11	130.6(9)	.	.	.	.	no
C14	C13	C15	C16	174.5(8)	.	.	.	.	no
N1	C13	C15	C16	-3.8(13)	.	.	.	.	no
C13	C15	C16	N2	9.7(13)	.	.	.	.	no
C13	C15	C16	C17	-165.8(8)	.	.	.	.	no
N2	C18	C19	C24	7.1(10)	.	.	.	.	no
C23	C18	C19	C20	-1.4(10)	.	.	.	.	no
N2	C18	C19	C20	-175.9(6)	.	.	.	.	no
C19	C18	C23	C27	179.3(7)	.	.	.	.	no
C19	C18	C23	C22	-1.4(10)	.	.	.	.	no
N2	C18	C23	C27	-6.3(10)	.	.	.	.	no
C23	C18	C19	C24	-178.5(6)	.	.	.	.	no



N2	C18	C23	C22	173.1(6)	.	.	.	.	no
C18	C19	C24	C25	-152.1(7)	.	.	.	.	no
C18	C19	C24	C26	82.4(9)	.	.	.	.	no
C20	C19	C24	C25	31.0(10)	.	.	.	.	no
C20	C19	C24	C26	-94.5(9)	.	.	.	.	no
C24	C19	C20	C21	-179.2(7)	.	.	.	.	no
C18	C19	C20	C21	3.8(11)	.	.	.	.	no
C19	C20	C21	C22	-3.2(13)	.	.	.	.	no
C20	C21	C22	C23	0.0(13)	.	.	.	.	no
C21	C22	C23	C18	2.1(12)	.	.	.	.	no
C21	C22	C23	C27	-178.5(8)	.	.	.	.	no
C18	C23	C27	C29	100.8(9)	.	.	.	.	no
C22	C23	C27	C28	48.3(10)	.	.	.	.	no
C18	C23	C27	C28	-132.3(8)	.	.	.	.	no
C22	C23	C27	C29	-78.5(10)	.	.	.	.	no
C31	C30	C35	C34	3.8(11)	.	.	.	.	no
C31	C30	C35	C36	-172.8(7)	.	.	.	.	no
Fe	C30	C35	C36	121.9(6)	.	.	.	.	no
Fe	C30	C31	C32	71.6(7)	.	.	.	.	no
C35	C30	C31	Fe	-71.1(7)	.	.	.	.	no
C35	C30	C31	C32	0.4(12)	.	.	.	.	no
Fe	C30	C35	C34	-61.5(6)	.	.	.	.	no
C30	C31	C32	C33	-3.7(11)	.	.	.	.	no
Fe	C31	C32	C33	62.1(6)	.	.	.	.	no
C31	C32	C33	C34	2.6(10)	.	.	.	.	no
C32	C33	C34	C35	1.9(11)	.	.	.	.	no
C33	C34	C35	C36	171.5(7)	.	.	.	.	no
C33	C34	C35	C30	-5.0(11)	.	.	.	.	no
C30	C35	C36	B	88.2(8)	.	.	.	.	no
C34	C35	C36	B	-88.2(9)	.	.	.	.	no
C35	C36	B	C49	-70.7(8)	.	.	.	.	no
C35	C36	B	C37	51.1(8)	.	.	.	.	no
C35	C36	B	C43	172.8(6)	.	.	.	.	no
B	C37	C38	F1	-5.9(10)	.	.	.	.	no
B	C37	C38	C39	172.5(7)	.	.	.	.	no
C38	C37	C42	F5	176.5(6)	.	.	.	.	no
C42	C37	C38	C39	2.4(10)	.	.	.	.	no
C38	C37	B	C43	151.4(7)	.	.	.	.	no
C38	C37	B	C49	35.2(9)	.	.	.	.	no
C42	C37	B	C36	81.3(8)	.	.	.	.	no
C38	C37	C42	C41	-3.9(10)	.	.	.	.	no
B	C37	C42	F5	6.1(10)	.	.	.	.	no
B	C37	C42	C41	-174.3(7)	.	.	.	.	no
C38	C37	B	C36	-87.7(8)	.	.	.	.	no
C42	C37	C38	F1	-176.0(6)	.	.	.	.	no
C42	C37	B	C43	-39.6(9)	.	.	.	.	no
C42	C37	B	C49	-155.8(6)	.	.	.	.	no
F1	C38	C39	F2	-3.1(10)	.	.	.	.	no
C37	C38	C39	C40	0.2(12)	.	.	.	.	no
C37	C38	C39	F2	178.5(7)	.	.	.	.	no
F1	C38	C39	C40	178.6(7)	.	.	.	.	no
F2	C39	C40	C41	-179.8(7)	.	.	.	.	no
F2	C39	C40	F3	2.4(12)	.	.	.	.	no
C38	C39	C40	C41	-1.6(12)	.	.	.	.	no
C38	C39	C40	F3	-179.3(7)	.	.	.	.	no
F3	C40	C41	F4	1.3(11)	.	.	.	.	no
C39	C40	C41	C42	0.1(11)	.	.	.	.	no
F3	C40	C41	C42	177.9(7)	.	.	.	.	no
C39	C40	C41	F4	-176.5(7)	.	.	.	.	no
F4	C41	C42	F5	-0.9(9)	.	.	.	.	no
C40	C41	C42	C37	2.9(11)	.	.	.	.	no
F4	C41	C42	C37	179.5(6)	.	.	.	.	no
C40	C41	C42	F5	-177.5(6)	.	.	.	.	no
B	C43	C44	C45	-174.4(7)	.	.	.	.	no

B	C43	C48	F10	-5.8(11)	.	.	.	.	no
C44	C43	C48	F10	-179.6(6)	.	.	.	.	no
C44	C43	C48	C47	1.3(11)	.	.	.	.	no
B	C43	C44	F6	5.4(10)	.	.	.	.	no
C44	C43	B	C49	86.4(8)	.	.	.	.	no
C48	C43	B	C36	36.0(10)	.	.	.	.	no
C48	C43	B	C37	151.9(7)	.	.	.	.	no
C48	C43	B	C49	-86.7(8)	.	.	.	.	no
B	C43	C48	C47	175.2(7)	.	.	.	.	no
C44	C43	B	C36	-150.9(7)	.	.	.	.	no
C44	C43	B	C37	-34.9(10)	.	.	.	.	no
C48	C43	C44	F6	179.4(6)	.	.	.	.	no
C48	C43	C44	C45	-0.4(11)	.	.	.	.	no
F6	C44	C45	F7	-0.9(10)	.	.	.	.	no
F6	C44	C45	C46	-179.2(7)	.	.	.	.	no
C43	C44	C45	F7	178.9(7)	.	.	.	.	no
C43	C44	C45	C46	0.6(12)	.	.	.	.	no
C44	C45	C46	F8	179.8(7)	.	.	.	.	no
C44	C45	C46	C47	-1.5(12)	.	.	.	.	no
F7	C45	C46	C47	-179.8(7)	.	.	.	.	no
F7	C45	C46	F8	1.5(12)	.	.	.	.	no
F8	C46	C47	C48	-179.0(7)	.	.	.	.	no
C45	C46	C47	F9	-179.3(7)	.	.	.	.	no
F8	C46	C47	F9	-0.7(11)	.	.	.	.	no
C45	C46	C47	C48	2.3(12)	.	.	.	.	no
F9	C47	C48	C43	179.3(7)	.	.	.	.	no
C46	C47	C48	F10	178.6(7)	.	.	.	.	no
F9	C47	C48	F10	0.3(10)	.	.	.	.	no
C46	C47	C48	C43	-2.3(12)	.	.	.	.	no
C50	C49	C54	F15	176.1(6)	.	.	.	.	no
B	C49	C54	F15	1.8(11)	.	.	.	.	no
B	C49	C54	C53	-179.0(7)	.	.	.	.	no
C50	C49	C54	C53	-4.6(11)	.	.	.	.	no
C50	C49	B	C37	37.3(10)	.	.	.	.	no
C50	C49	B	C43	-84.6(8)	.	.	.	.	no
C54	C49	B	C36	-32.3(10)	.	.	.	.	no
C54	C49	B	C37	-149.0(7)	.	.	.	.	no
C54	C49	B	C43	89.0(8)	.	.	.	.	no
C54	C49	C50	C51	3.9(11)	.	.	.	.	no
C50	C49	B	C36	154.0(7)	.	.	.	.	no
C54	C49	C50	F11	-177.5(6)	.	.	.	.	no
B	C49	C50	F11	-3.1(11)	.	.	.	.	no
B	C49	C50	C51	178.4(8)	.	.	.	.	no
F11	C50	C51	F12	0.9(11)	.	.	.	.	no
F11	C50	C51	C52	-179.8(7)	.	.	.	.	no
C49	C50	C51	F12	179.5(7)	.	.	.	.	no
C49	C50	C51	C52	-1.1(13)	.	.	.	.	no
C50	C51	C52	F13	-179.3(7)	.	.	.	.	no
C50	C51	C52	C53	-1.5(13)	.	.	.	.	no
F12	C51	C52	F13	0.0(13)	.	.	.	.	no
F12	C51	C52	C53	177.8(8)	.	.	.	.	no
F13	C52	C53	F14	-0.4(13)	.	.	.	.	no
C51	C52	C53	F14	-178.1(8)	.	.	.	.	no
C51	C52	C53	C54	0.9(13)	.	.	.	.	no
F13	C52	C53	C54	178.7(7)	.	.	.	.	no
C52	C53	C54	F15	-178.2(7)	.	.	.	.	no
C52	C53	C54	C49	2.5(13)	.	.	.	.	no
F14	C53	C54	F15	0.8(11)	.	.	.	.	no
F14	C53	C54	C49	-178.5(7)	.	.	.	.	no

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loop_
  _geom_contact_atom_site_label_1
  _geom_contact_atom_site_label_2
  _geom_contact_distance

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\_geom\_contact\_site\_symmetry\_1  
 \_geom\_contact\_site\_symmetry\_2  
 \_geom\_contact\_publ\_flag

Fe	C7	3.952(9)	.	.	no
Fe	C10	3.953(9)	.	.	no
Fe	C24	3.871(8)	.	.	no
Fe	C27	3.936(9)	.	.	no
Fe	C29	3.950(10)	.	.	no
Fe	F12	3.657(5)	.	4_554	no
Fe	H10	3.23(5)	.	.	no
Fe	H29	3.19(8)	.	.	no
Fe	H34	3.23(5)	.	.	no
Fe	H24	3.10(6)	.	.	no
F1	F2	2.644(6)	.	.	no
F1	F11	2.785(5)	.	.	no
F1	C30	3.345(8)	.	.	no
F1	C35	3.187(8)	.	.	no
F1	C49	2.822(9)	.	.	no
F1	C50	2.814(9)	.	.	no
F1	F7	2.892(5)	.	4_554	no
F2	F1	2.644(6)	.	.	no
F2	F3	2.722(6)	.	.	no
F2	C20	3.102(10)	.	6_545	no
F3	F4	2.730(6)	.	.	no
F3	F4	3.037(6)	.	7_556	no
F3	F2	2.722(6)	.	.	no
F3	C41	3.278(9)	.	7_556	no
F4	F3	2.730(6)	.	.	no
F4	F5	2.637(6)	.	.	no
F4	F3	3.037(6)	.	7_556	no
F4	C21	3.315(9)	.	7_556	no
F4	C33	3.248(8)	.	7_556	no
F4	C40	3.056(9)	.	7_556	no
F5	F6	2.811(6)	.	.	no
F5	C43	2.836(9)	.	.	no
F5	C17	3.045(10)	.	4_565	no
F5	F4	2.637(6)	.	.	no
F5	C44	2.875(9)	.	.	no
F6	C32	3.132(8)	.	4_555	no
F6	F5	2.811(6)	.	.	no
F6	F11	2.743(5)	.	.	no
F6	F7	2.642(6)	.	.	no
F6	C31	3.182(9)	.	4_555	no
F6	C37	2.813(8)	.	.	no
F6	C42	2.840(9)	.	.	no
F7	F8	2.726(7)	.	.	no
F7	C31	3.205(9)	.	4_555	no
F7	F1	2.892(5)	.	4_555	no
F7	F6	2.642(6)	.	.	no
F8	F7	2.726(7)	.	.	no
F8	F9	2.741(7)	.	.	no
F8	F13	2.943(6)	.	4_555	no
F8	C52	3.149(10)	.	4_555	no
F9	F10	2.619(6)	.	.	no
F9	F8	2.741(7)	.	.	no
F10	F9	2.619(6)	.	.	no
F10	C36	2.858(9)	.	.	no
F10	F15	2.944(5)	.	.	no
F11	F1	2.785(5)	.	.	no
F11	F6	2.743(5)	.	.	no
F11	F12	2.640(6)	.	.	no
F11	C38	2.863(8)	.	.	no
F11	C32	3.288(7)	.	4_555	no
F11	C37	2.838(8)	.	.	no

F12	F13	2.730(6)	.	.	no
F12	F11	2.640(6)	.	.	no
F12	Fe	3.657(5)	.	4_555	no
F12	C26	3.362(11)	.	4_555	no
F12	C15	3.301(9)	.	4_555	no
F13	F8	2.943(6)	.	4_554	no
F13	F12	2.730(6)	.	.	no
F13	F14	2.742(6)	.	.	no
F14	F13	2.742(6)	.	.	no
F14	F15	2.611(6)	.	.	no
F14	C12	3.245(12)	.	3_555	no
F15	C4	3.136(10)	.	.	no
F15	F14	2.611(6)	.	.	no
F15	C30	3.185(10)	.	.	no
F15	C5	3.287(9)	.	.	no
F15	F10	2.944(5)	.	.	no
F15	C36	2.902(9)	.	.	no
F2	H20	2.76(5)	.	6_545	no
F2	H26"	2.69(6)	.	6_545	no
F3	H29"	2.52(6)	.	7_556	no
F4	H33	2.53(5)	.	7_556	no
F5	H17"	2.85(7)	.	4_565	no
F5	H17	2.47(7)	.	4_565	no
F6	H32	2.59(5)	.	4_555	no
F6	H31	2.69(6)	.	4_555	no
F6	H21	2.79(7)	.	7_556	no
F7	H28'	2.73(8)	.	4_565	no
F8	H9'	2.26(9)	.	4_565	no
F9	H9	2.73(7)	.	4_565	no
F9	H14"	2.82(5)	.	4_565	no
F10	H36'	2.83(6)	.	.	no
F10	H36	2.25(6)	.	.	no
F11	H25'	2.74(7)	.	4_555	no
F11	H24	2.86(5)	.	4_555	no
F11	H32	2.56(5)	.	4_555	no
F12	H24	2.79(5)	.	4_555	no
F12	H26	2.66(14)	.	4_555	no
F14	H12	2.82(7)	.	3_555	no
F15	H30	2.48(7)	.	.	no
F15	H36	2.26(6)	.	.	no
N1	H7	2.59(7)	.	.	no
N1	H10	2.42(5)	.	.	no
N2	H24	2.49(6)	.	.	no
N2	H26	2.75(14)	.	.	no
N2	H27	2.49(5)	.	.	no
C2	C14	3.471(11)	.	.	no
C4	F15	3.136(10)	.	.	no
C5	F15	3.287(9)	.	.	no
C6	C30	3.582(11)	.	.	no
C6	C14	3.421(12)	.	.	no
C7	C13	3.406(11)	.	.	no
C7	Fe	3.952(9)	.	.	no
C9	C14	3.548(16)	.	3_565	no
C10	Fe	3.953(9)	.	.	no
C12	C52	3.546(16)	.	4_554	no
C12	F14	3.245(12)	.	3_555	no
C13	C7	3.406(11)	.	.	no
C14	C6	3.421(12)	.	.	no
C14	C2	3.471(11)	.	.	no
C14	C9	3.548(16)	.	3_565	no
C15	F12	3.301(9)	.	4_554	no
C16	C27	3.341(11)	.	.	no
C16	C24	3.598(11)	.	.	no
C17	C19	3.560(12)	.	.	no

C17	C27	3.546(13)	.	.	no
C17	F5	3.045(10)	.	4_564	no
C17	C26	3.549(13)	.	.	no
C17	C23	3.320(12)	.	.	no
C18	C33	3.299(9)	.	.	no
C19	C33	3.245(10)	.	.	no
C19	C17	3.560(12)	.	.	no
C20	F2	3.102(10)	.	6_555	no
C21	C41	3.444(11)	.	7_556	no
C21	F4	3.315(9)	.	7_556	no
C23	C17	3.320(12)	.	.	no
C24	C33	3.577(10)	.	.	no
C24	Fe	3.871(8)	.	.	no
C24	C16	3.598(11)	.	.	no
C24	C32	3.403(11)	.	.	no
C25	C32	3.547(13)	.	.	no
C26	C17	3.549(13)	.	.	no
C26	F12	3.362(11)	.	4_554	no
C27	Fe	3.936(9)	.	.	no
C27	C17	3.546(13)	.	.	no
C27	C16	3.341(11)	.	.	no
C28	C45	3.582(13)	.	4_564	no
C29	Fe	3.950(10)	.	.	no
C30	C6	3.582(11)	.	.	no
C30	C54	3.491(12)	.	.	no
C30	F15	3.185(10)	.	.	no
C30	C49	3.565(10)	.	.	no
C30	F1	3.345(8)	.	.	no
C31	F6	3.182(9)	.	4_554	no
C31	F7	3.205(9)	.	4_554	no
C32	F11	3.288(7)	.	4_554	no
C32	F6	3.132(8)	.	4_554	no
C32	C24	3.403(11)	.	.	no
C32	C25	3.547(13)	.	.	no
C33	C24	3.577(10)	.	.	no
C33	F4	3.248(8)	.	7_556	no
C33	C19	3.245(10)	.	.	no
C33	C18	3.299(9)	.	.	no
C34	C38	3.103(10)	.	.	no
C34	C37	3.138(11)	.	.	no
C34	C42	3.588(11)	.	.	no
C35	C38	3.203(10)	.	.	no
C35	F1	3.187(8)	.	.	no
C36	F15	2.902(9)	.	.	no
C36	F10	2.858(9)	.	.	no
C37	C34	3.138(11)	.	.	no
C37	F6	2.813(8)	.	.	no
C37	F11	2.838(8)	.	.	no
C38	C35	3.203(10)	.	.	no
C38	F11	2.863(8)	.	.	no
C38	C34	3.103(10)	.	.	no
C38	C50	3.315(11)	.	.	no
C40	F4	3.056(9)	.	7_556	no
C40	C41	3.557(12)	.	7_556	no
C41	C40	3.557(12)	.	7_556	no
C41	F3	3.278(9)	.	7_556	no
C41	C21	3.444(11)	.	7_556	no
C42	C34	3.588(11)	.	.	no
C42	F6	2.840(9)	.	.	no
C42	C44	3.321(12)	.	.	no
C43	F5	2.836(9)	.	.	no
C44	C42	3.321(12)	.	.	no
C44	F5	2.875(9)	.	.	no
C45	C28	3.582(13)	.	4_565	no

C49	C30	3.565(10)	.	.	no
C49	F1	2.822(9)	.	.	no
C50	F1	2.814(9)	.	.	no
C50	C38	3.315(11)	.	.	no
C52	F8	3.149(10)	.	4_554	no
C52	C12	3.546(16)	.	4_555	no
C54	C30	3.491(12)	.	.	no
C1	H14	2.24(7)	.	.	no
C2	H14	2.84(7)	.	.	no
C3	H9"	2.89(11)	.	.	no
C3	H8	2.65(7)	.	.	no
C4	H4	3.07(7)	.	2_555	no
C5	H11	3.08(15)	.	.	no
C5	H12	3.00(7)	.	.	no
C5	H11"	2.79(6)	.	.	no
C6	H30	3.05(7)	.	.	no
C6	H14	2.58(7)	.	.	no
C8	H3	2.67(6)	.	.	no
C8	H15	2.77(5)	.	4_565	no
C8	H29'	3.06(10)	.	.	no
C9	H3	2.97(5)	.	.	no
C11	H5	2.86(7)	.	.	no
C12	H5	3.02(7)	.	.	no
C12	H14	3.07(7)	.	.	no
C13	H10	3.02(5)	.	.	no
C13	H7	2.77(7)	.	.	no
C14	H12"	2.90(8)	.	.	no
C14	H9	2.78(8)	.	.	no
C16	H26	2.61(14)	.	.	no
C16	H27	2.66(5)	.	.	no
C17	H27	2.96(5)	.	.	no
C17	H26	2.70(14)	.	.	no
C18	H26	3.00(13)	.	.	no
C18	H17"	2.57(7)	.	.	no
C19	H17"	3.04(7)	.	.	no
C19	H33	2.86(5)	.	.	no
C20	H25	3.02(5)	.	.	no
C20	H25"	2.93(5)	.	.	no
C20	H33	3.08(5)	.	.	no
C22	H29"	2.94(7)	.	.	no
C22	H28	2.85(6)	.	.	no
C22	H25"	2.90(6)	.	6_555	no
C24	H32	2.98(5)	.	.	no
C25	H32	2.78(6)	.	.	no
C25	H22	2.71(10)	.	6_545	no
C25	H20	2.56(5)	.	.	no
C26	H17"	3.03(7)	.	.	no
C28	H22	2.70(10)	.	.	no
C31	H11	3.05(14)	.	.	no
C32	H25"	3.08(6)	.	.	no
C32	H24	2.76(5)	.	.	no
C34	H29	2.94(8)	.	.	no
C36	H8"	3.04(7)	.	.	no
C37	H34	2.94(5)	.	.	no
C44	H31	3.03(6)	.	4_555	no
C45	H28'	3.01(8)	.	4_565	no
C48	H36	3.01(5)	.	.	no
C52	H12'	2.91(6)	.	4_555	no
C53	H12'	2.90(6)	.	4_555	no
C54	H30	2.91(7)	.	.	no
C54	H36	3.02(6)	.	.	no
H3	C8	2.67(6)	.	.	no
H3	C9	2.97(5)	.	.	no
H3	H8	2.07(9)	.	.	no

H3	H9"	2.50(12)	.	.	no
H3	H3	2.48(8)	.	2_555	no
H4	C4	3.07(7)	.	2_555	no
H4	H4	2.53(9)	.	2_555	no
H5	C11	2.86(7)	.	.	no
H5	C12	3.02(7)	.	.	no
H5	H11"	2.33(9)	.	.	no
H7	N1	2.59(7)	.	.	no
H7	C13	2.77(7)	.	.	no
H8	C3	2.65(7)	.	.	no
H8	H3	2.07(9)	.	.	no
H8	H9"	2.23(12)	.	.	no
H8'	H9'	2.53(12)	.	.	no
H8'	H29'	2.26(13)	.	.	no
H8"	C36	3.04(7)	.	.	no
H8"	H36	2.50(9)	.	.	no
H9	C14	2.78(8)	.	.	no
H9	H14"	2.30(10)	.	.	no
H9	F9	2.73(7)	.	4_564	no
H9'	H8'	2.53(12)	.	.	no
H9'	F8	2.26(9)	.	4_564	no
H9"	C3	2.89(11)	.	.	no
H9"	H3	2.50(12)	.	.	no
H9"	H8	2.23(12)	.	.	no
H10	Fe	3.23(5)	.	.	no
H10	N1	2.42(5)	.	.	no
H10	C13	3.02(5)	.	.	no
H11	C5	3.08(15)	.	.	no
H11	C31	3.05(14)	.	.	no
H11'	H12'	2.48(10)	.	.	no
H11"	C5	2.79(6)	.	.	no
H11"	H5	2.33(9)	.	.	no
H11"	H12	2.59(9)	.	3_555	no
H12	C5	3.00(7)	.	.	no
H12	F14	2.82(7)	.	3_555	no
H12	H11"	2.59(9)	.	3_555	no
H12'	H11'	2.48(10)	.	.	no
H12'	C52	2.91(6)	.	4_554	no
H12'	C53	2.90(6)	.	4_554	no
H12"	C14	2.90(8)	.	.	no
H12"	H14	2.45(10)	.	.	no
H12"	H14'	2.59(11)	.	.	no
H14	C1	2.24(7)	.	.	no
H14	C2	2.84(7)	.	.	no
H14	C6	2.58(7)	.	.	no
H14	C12	3.07(7)	.	.	no
H14	H12"	2.45(10)	.	.	no
H14'	H12"	2.59(11)	.	.	no
H14"	H9	2.30(10)	.	.	no
H14"	H15	2.56(8)	.	.	no
H14"	F9	2.82(5)	.	4_564	no
H15	H14"	2.56(8)	.	.	no
H15	H17'	2.09(10)	.	.	no
H15	C8	2.77(5)	.	4_564	no
H17	F5	2.47(7)	.	4_564	no
H17'	H15	2.09(10)	.	.	no
H17"	C18	2.57(7)	.	.	no
H17"	C19	3.04(7)	.	.	no
H17"	C26	3.03(7)	.	.	no
H17"	H26	2.45(15)	.	.	no
H17"	F5	2.85(7)	.	4_564	no
H20	C25	2.56(5)	.	.	no
H20	H25	2.36(7)	.	.	no
H20	H25"	2.59(7)	.	.	no

H20	F2	2.76(5)	.	6_555	no
H21	F6	2.79(7)	.	7_556	no
H22	C28	2.70(10)	.	.	no
H22	H28	2.18(11)	.	.	no
H22	C25	2.71(9)	.	6_555	no
H22	H25"	2.07(11)	.	6_555	no
H24	Fe	3.10(6)	.	.	no
H24	N2	2.49(6)	.	.	no
H24	C32	2.76(5)	.	.	no
H24	H32	2.42(7)	.	.	no
H24	F11	2.86(5)	.	4_554	no
H24	F12	2.79(5)	.	4_554	no
H25	C20	3.02(5)	.	.	no
H25	H20	2.36(7)	.	.	no
H25	H26"	2.59(7)	.	.	no
H25	H28	2.56(8)	.	6_545	no
H25'	H26'	2.34(8)	.	.	no
H25'	F11	2.74(7)	.	4_554	no
H25"	C20	2.93(5)	.	.	no
H25"	C32	3.08(6)	.	.	no
H25"	H20	2.59(7)	.	.	no
H25"	H32	2.39(8)	.	.	no
H25"	H33	2.45(8)	.	.	no
H25"	C22	2.90(5)	.	6_545	no
H25"	H22	2.07(11)	.	6_545	no
H26	N2	2.75(14)	.	.	no
H26	C16	2.61(14)	.	.	no
H26	C17	2.70(14)	.	.	no
H26	C18	3.00(13)	.	.	no
H26	H17"	2.45(15)	.	.	no
H26	F12	2.66(14)	.	4_554	no
H26'	H25'	2.34(8)	.	.	no
H26"	H25	2.59(7)	.	.	no
H26"	F2	2.69(6)	.	6_555	no
H27	N2	2.49(5)	.	.	no
H27	C16	2.66(5)	.	.	no
H27	C17	2.96(5)	.	.	no
H28	C22	2.85(6)	.	.	no
H28	H22	2.18(11)	.	.	no
H28	H25	2.56(8)	.	6_555	no
H28'	H29'	2.59(12)	.	.	no
H28'	F7	2.73(8)	.	4_564	no
H28'	C45	3.01(8)	.	4_564	no
H29	Fe	3.19(8)	.	.	no
H29	C34	2.94(8)	.	.	no
H29	H34	2.60(10)	.	.	no
H29'	C8	3.06(10)	.	.	no
H29'	H8'	2.26(13)	.	.	no
H29'	H28'	2.59(12)	.	.	no
H29"	C22	2.94(7)	.	.	no
H29"	F3	2.52(6)	.	7_556	no
H30	F15	2.48(7)	.	.	no
H30	C6	3.05(7)	.	.	no
H30	C54	2.91(7)	.	.	no
H30	H36	2.48(8)	.	.	no
H31	F6	2.69(6)	.	4_554	no
H31	C44	3.03(6)	.	4_554	no
H32	C24	2.98(5)	.	.	no
H32	C25	2.78(6)	.	.	no
H32	H24	2.42(7)	.	.	no
H32	H25"	2.39(8)	.	.	no
H32	F6	2.59(5)	.	4_554	no
H32	F11	2.56(5)	.	4_554	no
H33	C19	2.86(5)	.	.	no



H33	C20	3.08(5)	.	.	no
H33	H25"	2.45(8)	.	.	no
H33	F4	2.53(5)	.	7_556	no
H34	Fe	3.23(5)	.	.	no
H34	C37	2.94(5)	.	.	no
H34	H29	2.60(10)	.	.	no
H34	H36'	2.40(9)	.	.	no
H36	F10	2.25(6)	.	.	no
H36	F15	2.26(6)	.	.	no
H36	C48	3.01(5)	.	.	no
H36	C54	3.02(6)	.	.	no
H36	H8"	2.50(9)	.	.	no
H36	H30	2.48(8)	.	.	no
H36'	F10	2.83(6)	.	.	no
H36'	H34	2.40(9)	.	.	no

loop\_

\_geom\_hbond\_atom\_site\_label\_D:wq

\_geom\_hbond\_atom\_site\_label\_H

\_geom\_hbond\_atom\_site\_label\_A

\_geom\_hbond\_distance\_DH

\_geom\_hbond\_distance\_HA

\_geom\_hbond\_distance\_DA

\_geom\_hbond\_angle\_DHA

\_geom\_hbond\_site\_symmetry\_A

\_geom\_hbond\_publ\_flag

#

#D H A D - H H...A D...A D - H...A symm(A)

#

C9	H9'	F8	1.31(10)	2.26(9)	3.535(13)	162(6)	4_564	yes
C10	H10	N1	0.93(6)	2.42(5)	2.984(11)	119(4)	.	yes
C17	H17	F5	0.93(7)	2.47(7)	3.045(10)	120(5)	4_564	yes
C24	H24	N2	0.96(6)	2.49(6)	2.913(10)	107(4)	.	yes
C27	H27	N2	0.82(5)	2.49(5)	2.938(10)	115(5)	.	yes
C29	H29"	F3	1.02(7)	2.52(6)	3.419(11)	147(4)	7_556	yes
C30	H30	F15	0.83(7)	2.48(7)	3.185(10)	143(6)	.	yes
C33	H33	F4	1.09(6)	2.53(5)	3.248(8)	123(3)	7_556	yes
C36	H36	F10	1.05(6)	2.25(6)	2.858(9)	115(4)	.	yes
C36	H36	F15	1.05(6)	2.26(6)	2.902(9)	118(4)	.	yes

#===END of Crystallographic Information File